Official Transcript of Proceedings

NUCLEAR REGULATORY COMMISSION

Title:	Advisory Committee on Nuclear Waste 165th Meeting
Docket Number:	(not applicable)
Location:	Rockville, Maryland
Date:	Tuesday, November 15, 2005

Work Order No.: NRC-742 Pages 1-166

NEAL R. GROSS AND CO., INC.
Court Reporters and Transcribers
1323 Rhode Island Avenue, N.W.
Washington, D.C. 20005
(202) 234-4433

UNITED STATES OF AMERICA

NUCLEAR REGULATORY COMMISSION

\+ + + + +

ADVISORY COMMITTEE ON NUCLEAR WASTE (ACNW)

165TH MEETING

\+ + + + +

TUESDAY,

NOVEMBER 15, 2005

\+ + + + +

ROCKVILLE, MARYLAND

\+ + + + +

The Advisory Committee met at 8:30 a.m. in Room T-2B3 of the Nuclear Regulatory Commission, Two White Flint North, 11545 Rockville Pike, Rockville, Maryland, Dr. Michael T. Ryan, Chairman, presiding.

MEMBERS PRESENT:

MICHAEL T. RYAN, Chairman
ALLEN G. CROFF, Vice Chairman
JAMES H. CLARKE, Member
WILLIAM J. HINZE, Member
RUTH F. WEINER, Member

ACNW STAFF PRESENT:

NEIL M. COLEMAN
LATIF HAMDAN
RICHARD K. MAJOR
SHARON A. STEELE
MICHAEL LEE

ALSO PRESENT:

SUSAN ALTMAN, Sandia
RANDALL CYGAN, Sandia
JIM LIEBERMAN, Consultant
TODD LOVINGER
BRUCE MARSH, ACNW Consultant
BILL OTT
JOHN FLACK, ACNW

I N D E X

P R O C E E D I N G S

8:51 A.M.

CHAIRMAN RYAN: The meeting will come to order. This is the second day of the 165th meeting of the Advisory Committee on Nuclear Waste. My name is Michael Ryan, Chairman of the ACNW. The other Members of the Committee present are Vice Chairman Alan Croff, Ruth Weiner, James Clarke and William Hinze.

During today's meeting, the Committee will hear a briefing by and hold discussions with representatives of the Office of Nuclear Regulatory Research on radionuclide sorption in soils and its impact on reactive transport. We'll make preparations for the Commission briefing on January 11, 2006 and we'll hear presentations and hold discussions with representatives of the U.S. Geological Survey and the Office of Research regarding demonstrations of the generalized composite approach to modeling reactor transport.

We will discuss the Committee's draft white paper on low-level radioactive waste and discuss draft committee letters and reports.

This meeting is being conducted in accordance with the provisions of the Federal Advisory Committee Act. Mr. Alan Pasternak of the California

Radiation Forum will be participating by phone during discussion of the low-level waste white paper.

It is requested that speakers use one of the microphones, identify themselves and speak with sufficient clarity and volume so that they can be readily heard. It is also requested that if you have cell phones or pagers that you kindly turn them off. Thank you very much.

I have one item with regard to staff that I'd like to bring to everybody's attention. Ms. Jesse Delgado of the Advisory Committee on Reactor Safeguards and Advisory Committee on Reactor Waste was honored at the Hispanic Employment Program Advisory Committee dinner last week. Jesse received this year's Equal Employment Opportunity Award, co-sponsored by the Office of Small Business and Civil Rights and the KEPAC organization for her outstanding service over a number of years. The EEO award is presented in recognition of outstanding contributions to the advancement of equal employment goals and for promoting diversity within the Nuclear Regulatory Commission.

Jesse, we congratulate you on this recognition and I'd like to make that part of the record.

(Applause.)

Thank you very much for all that you do and all that's ahead and we appreciate your service. Thank you very much.

With that, I will turn over the gavel to Ruth Weiner who will be leading us through the two presentation sections today.

MEMBER WEINER: Thank you, Mr. Chairman. This morning we're going to have several presentations on research on reactive transport and I'm going to ask Bill Ott from the Office of Nuclear Regulatory Research to lead off and to introduce our speakers.

Do you want to speak from back there, Bill?

MR. OTT: This will be fine.

CHAIRMAN RYAN: Just for the reporter, if you will identify yourself and who you're with. NRC is fine and then every other speaker do the same, and that will be great. Thanks.

MR. OTT: Okay, I'm Bill Ott. I'm from the -- I'm a section chief in the Office of Nuclear Regulatory Research for the Nuclear Regulatory Commission.

And just one minor correction. Ruth knows Jim Davis couldn't be with us today, so the afternoon session is actually not going to take place. We're going to extend the morning session a little bit and cover a little bit of what Jim was going to deal with with regard to the OACD Nuclear Energy Agency. I'll do that presentation.

Hopefully, if it meets with your schedule and Jim's, we can bring them in in December, to talk about the Naturita Project which is really the second phase of this work that we're talking about today.

And basically what we're talking about today is how we deal with chemical interactions in soils with graduated radionuclide transport processes. It's been a thorn in the side of PA modelers for years and we've extended considerable effort in trying to come to grips with this problem and we're going to talk to you about some of those efforts that we've put forth today.

First talk is going to be Randy, presenting something that Jim Davis and he collaborated on with regard to sort of an overview of the research that we've been putting together. Then Randy, Randy Cygan and Susan Altman will present the work that's been done by Sandia and will give you a fairly detailed overview of that work. They'll end with a discussion of the MOU which was -- there's a

Memorandum of Understanding with many federal agencies dealing with multi-media environmental modeling, research and development of those models. And we have a working group on reactive transport. We had a major workshop about a year ago and they're going to discuss the results of that workshop.

The next presentation was supposed to be Jim Davis. That's not going to happen and then I'll end up this morning with a discussion of the NEA sorption project which is an international effort that's been trying to deal with the sorption effort.

With that, I'll turn it over to Randy Cygan.

Randy?

MR. CYGAN: Does the Committee prefer that I sit? I'd rather stand or --

CHAIRMAN RYAN: We'll have to get a lapel microphone for you, if we do that and you're welcome to do it any way you're comfortable.

MR. CYGAN: I should be much more comfortable standing, if you don't mind.

CHAIRMAN RYAN: You need a microphone. We're recording.

MR. CYGAN: I assume you can hear me? Okay. Randy Cygan, Sandia National Labs for the record. Thank you, Mr. Chairman, Dr. Weiner and the rest of the Committee Members.

I appreciate this opportunity to present our summary of our studies, the results of our work this morning. Sort of just recently we learned about Jim Davis not being able to attend today, so Jim was able to e-mail me some introductory slides. I got them on Saturday and I'm going to present them now. These were prepared by Jim, and hopefully I'll be able to represent best as I can some of the findings.

They're really meant to be an overview of where all of our projects fit together. It's sort of how they dovetail together and relate to performance assessment for looking at either decommissioning of nuclear power plants or dealing with nuclear waste sites, mining, tailing operations and that sort of thing.

We all agree, at least in the geochemistry discipline, the critical need for understanding how radionuclides migrate through the environment. We're most concerned, the USGS and Sandia were most concerned with sorption processes and trying to understand how we can best describe the chemistry and then transfer those into reactive transport modeling and hydrologic transport codes that eventually get the answer, if you will, with regards to performance assessment, ultimately the dose rate that eventually goes into the water supply, for example.

So we do have some issues about making this combination, just ground water flow mixing in flow environments, fractured flow, porous media flow. We know that there are some concerns across the extensive parameters of being pH, carbon dioxide content, these partial pressures, radionuclides concentration, temperature, ionic strength and so on.

Throughout the presentations this morning, you'll hear a lot more of these details being brought out, but in this overview, what we're trying to do is combine the more standard approach, combine it with very detailed chemistry and try to get a fairly generalized and detailed reactive transport model that's presented here, essentially looking at concentration profiles, a radioactive plume that goes downstream from the source. And then trying to incorporate that, as I said, into performance assessment.

To back up a few steps, to give you an idea of what's involved in looking at the thermodynamics, trying to generalize the thermodynamics to better look at sorption processes, typically, we always -- geochemists will go back to just looking at standard solubilities and this is a plot of the law of concentration of some aqueous species as a function of pH. Thee's a fairly narrow pH range from 5 to 7.5. This is showing you the solubility curve for schoepite, a uranium ore.

Essentially, this dotted line represents that solubility curve, knowing that at low pHs we have higher solubility. Middle range, it drops. Greater solubility off on the right, but underneath this solubility line, this limit, are a set of lines that describe the speciation in this aqueous solution, above the uranium materials that can come out when you dissolve the schoepite. These range from uranium -- uranyl sulphate, uranyl oxide, the standard uranyl cadion and then as you go up to higher pHs, especially where you have CO_2 being involved in the reactions, you start to form these quite stable uranyl carbonate complexes. But this is the standard approach aqueous geochemists having been using to just look at solubility limits and what the speciation might be.

Now these details are quite important, especially at the high pH ranges where we start to form these carbonate complexes. And you'll see later on how critical they are.

Now we also have the availability to look at the speciation across pH range and how it varies each of these species. What we have here is an overview, an overlay of all the different compounds: low pH, typically uranyl; middle pH range, we have these hydroxides that come out as species and then again as I'm repeating, the carbonate complexes is at the high pH. You start to see this trace of these curves and they sort of map out what I showed on the previous slide for the solubility of schoepite.

Now that's the standard geochemical thermodynamic approach, knowing that we have a solid phase that can dissolve and precipitate, if you will. We have species that occur in solution as a result of that dissolution and we're taking that one step further. And throughout the rest of the presentation you'll be hearing more and more about how the solids come into play and what are the sorption processes that occur on these solids.

And this is a representation of hematite and what we're able to see using some fairly advanced analytical methods, specifically extended x-ray fine structure, absorption fine structure ex-outs, you can get the details of what a sorption complex might be. And we know from those studies that we can form a uranyl(VI) carbonate complex right on the edge of this particular polyhedron representation, the octohedran in hematite. So this is a very fine detail that we're getting. And what we're trying to do is combine these data to develop the reactive transport models.

This is a set of results now for uranyl complexes on hematite and you can see the detail. You get the coordination of the uranyl group. It's coordination with carbonate groups, other oxygens, and then with the substrate itself, the iron oxide.

So in the first part of the slide you essentially see the thermodynamics, how you would write an association constant, an equilibrium constant for how uranyl will complex with sulphite in this example. This is an aqueous solution. Simple K is just the concentration of the complex divided by the reactives. Okay?

Now when you have a substrate and you start to look at the association of these complexes or some subset of those complexes with the substrate, you can write very similar thermodynamically grounded reactions as well. Here we have a mineral surface, in this case it's an iron oxide reacting with the uranyl (VI) cadion and with water and you form this now stable sorption complex here, represented on the right.

And just like you would for the aqueous system, you could write a sorption reaction here and an equilibrium constant. We're using fundamental thermodynamics now, using mass action laws to understand now surface species, analogous as you would with solution complexes.

Now this is just a repeat of the previous slide, but we want to know that when you write these Ks you also have Ks that are involved with the aqueous solution, so what we want to look at is what's going on in the solution and how it might affect the uranyl concentration here. And I could step up in this slide and you can start to see now that we have a set of mass action laws, a set of equilibrium constants that now will affect, for example, the carbonate concentration in this system. And we know that the uranyl will be reacting with the carbonate to form these, for example, these type of complexes and solution.

And this rigorous description of the thermodynamics will control ultimately how much uranyl is now going to be available to form these complexes. The point I'm trying to make here or I should say the point that Jim's trying to make here is that it's not a simple Kd. It's a very complicated chemical system that you're trying to describe and a Kd may work in some cases, but it's just not going to work if you want to be rigorous and general in describing how uranyl will sorb, for example.

This is an example if you take it one further step going into a reactive model where you look at a breakthrough curve for let's say a plume going downstream. In one case, you might have a sorbing solute, some substrate here that's going to be reacting with some component. And the blue case, it's a nonreactive tracer, so obviously this guy is going to be going downstream and not sorbing, whereas this guy is going to be sorbing and you could use the classic Kd to describe it. There is a retardation factor that's involved here in how you might attenuate the transport of the sorbing solute.

But we know and I'll be showing you example of how variable that result will be if you start to compare Kd with the more rigorous thermodynamic sorption model. Jim uses TSM to describe that as thermodynamic sorption model. I'll be using SCM, surface complexation model to look at the specifics of how you describe the sorption.

This past slide is sort of a general

slide, showing you the different levels of complexity, as you go from a simple KD model which is very typical of performance assessment codes, where you have a fairly simple chemistry, constant chemistry and a simple linear absorption. You could step up a little bit by looking at isotherms, nonlinear isotherms such as a Freundlick and then what we're proposing and all the studies that you'll be hearing later about variable chemistry where we have aqueous reactions that are involved with the sorption reactions much more sophisticated approach, but in this case we have the fractionation being represented as a function of chemistry, so these are the TSMs.

So obviously in the bottom slide, demonstrate how TSM can benefit PA by increasing the scientific credibility and reducing uncertainty in representation of the sorption process and I think that's a nice little summary statement that Jim has generated, just demonstrating that if we spend the effort, look at the chemistry, try to generalize it, be thermodynamically solid in how you evaluate it, you can get a much better description of sorption. You could allow all the variables to be introduced and understand those variables and how they influence sorption. And this way you could also reduce the uncertainty.

Now I'm going to step into the next presentation. I don't object to having questions in the middle of the presentation. What does the Committee --

MEMBER WEINER: I was just going to ask if the Committee has any questions now.

MEMBER CLARKE: Randy, this may becoming up. So far everything you've been talking about is equilibrium sorption, is that correct?

MR. CYGAN: Yes.

MEMBER CLARKE: Are you doing any non-equilibrium work at all?

MR. CYGAN: There are ways to introduce the non-equilibrium component, trying to get kinetic factors in there. Those have been introduced at some level of sophistication. As you probably know, we have difficulty with even thermodynamic parameters. Kinetic factors parameters, reaction rates are much more difficult to ascertain, either experimentally or from theory.

We do have the structure together to incorporate them, but there's some hesitancy in just automatically dumping in parameters.

MEMBER CLARKE: I understand.

MR. CYGAN: So yes, some studies have been done and quite successfully, but I'm not going to be presenting those in this morning's presentation.

MEMBER CLARKE: Fair enough, thank you.

MR. CYGAN: That's a good question.

MEMBER HINZE: Randy, what is the order of magnitude of the difference when you consider the thermodynamic model versus a simple Kd? What kinds of orders of magnitude are we working with?

MR. CYGAN: I'll be showing you in a second some examples of what that comparison might be, but there are some where they're in fairly good agreement within an order of magnitude, for example, some factor, wherein in other cases you might see many orders of magnitude comparing Kd to the thermodynamic model. But it's so site specific on application.

MEMBER HINZE: What about other variables, temperature and the like? Are these affecting the results in a meaningful way?

MR. CYGAN: Oh certainly. You could use the structured thermodynamic approach to look at heat capacity effects and anthalpies and how they might influence some of these constants, some of the thermodynamic parameters. A lot of systems, we know these values quite well and we could easily extrapolate from the room temperature values for reaction constant. We could certainly get them scaled up to the right temperature for the application. Our reactive transport models often are polythermal, going through several different temperature excursions and we have a good feel for a lot of the parameters, how they vary with temperature and so there is some consistency there.

With sorption data, there's some uncertainty with regards to higher temperature extrapolations, but there are a handful of people. We're not doing this work, but I know there are several groups that are looking into how high temperature processes will affect sorption.

MEMBER HINZE: And these are effective both in the unsaturated as well as the saturated zone?

MR. CYGAN: Yes. In fact, part of the MOU, one of the findings of the MOU and our workshop from last year is to essentially start looking at betyl zone scenarios, trying to get a better feel of the saturation rate and looking at the cyclic nature of wetting and that sort of thing.

MEMBER HINZE: That will be interesting.

CHAIRMAN RYAN: I guess I'm thick in the head for the day. I'm kind of interested in the certainty or uncertainty questions and when I hear that -- and measurement, I guess. You know, what do you measure and what are you calculating and how does this improve my ability to really tease out what is risk significant?

Don't answer that necessarily with your introductory stuff, but I would be kind of interested in how this view of transport will give me a better insight into what's moving where, when so I can then have a better estimate of ultimate risk from that activity. I understand it has its own merit as the science of transport, but I want to think about and I always think about well, does this help me to make a better dose estimate.

MR. CYGAN: It comes down to a philosophical question in some cases when we start to look at some of these sensitivity and uncertainty analyses and you'll see some examples that might help explain that better, but yeah, when you try to look at how all these different parameters, especially if some are parameterized from empirical measurements, it's interesting to see how those areas are propagated down the radionuclide, the path and then ultimately to dose.

CHAIRMAN RYAN: Sure.

MR. CYGAN: That's a critical question, obviously for PA.

CHAIRMAN RYAN: And I think from my point of view and perhaps the Committee's focus is that's probably the critical value of these kinds of improvements, if we can do a better job of performance assessment or risk-informed performance assessment.

So just the thought as you and the other speakers come along that those kind of questions are on my mind.

MR. CYGAN: We'll be addressing them. You'll see shortly some examples.

CHAIRMAN RYAN: Great. Thanks.

MEMBER WEINER: Any of the staff have any questions at this point?

Go ahead then, Randy.

MR. CYGAN: Okay, now I'm going to switch to specifically the Sandia effort. And I'll be leading off and then Susan Altman will be following me on some of the characterization studies.

Specifically, the contract --

MEMBER WEINER: Before you start, could you tell us what JCN is?

MR. CYGAN: That's a good question for my NRC manager, I guess.

MR. OTT: Job Control Number.

MEMBER WEINER: Thank you.

MR. CYGAN: We were working with JCN for so long, it's sort of one of these things you just accept. We've been working on JCN for the last three years, this particular JCN. We've been funded previously through contracts with the NRC. Our earlier work has always -- well, we've always been looking at sorption processes and we did a lot more lab benchwork during that previous and I'll mention it briefly coming up here.

Actually, here it is. Here's another JCN, the W6811. In that effort, we were looking at more lab bench based analysis of sorption. We were looking at sorption of cesium, sorption of strontium, looking at their behavior on goethite, ferrihydrite. We also did some theoretical work for that effort and ultimately what came out of that were four summary NUREG reports and there are a handful of journal articles and book -- articles in books that related specifically to sorption.

The present one we started in July 2002, we met all these deliverables since right now we're under -- I forgot the term -- no cost extension. We are in the midst now of writing up a lot of our studies, trying to finish those in terms of journal articles, but we submitted all of our NUREG reports.

I took this directly from our original 189, the proposal for the current project and obviously, I don't want to read it, but I think it's a very good description of why we want to get beyond the Kd approach and what the projects' objectives were.

In this effort, what we were trying to do though is get beyond the Kd generalized sorption models. We had a task that's related to looking at the uncertainty as brought up by the Chairman, looking at how the uncertainty and sorption parameters will ultimately affect what's observed downstream, for example, the evolution of a contaminant plume. We have a component that Susan is going to be describing shortly on the characterization of sorption in soils, complex soils, mineral mixtures. And then we also had a theoretical effort that involves molecular modeling which might be the more unusual approach to looking at sorption and I'll be presenting that next.

I guess this is just a summary of the formal tasks. Task 1 was the work plan. Molecular modeling is Task 2. We're looking at uranyl and cesium. There was a probabilistic approach; and characterization, and then finally our last task was added on about two years ago and this is related to the interagency MOU and related to also our workshop that was held in Albuquerque.

In terms of deliverables, these are some recent NUREG reports that came out. The starred entries are the topical reports that were required under our contract and those were delivered just recently. I can provide hard copies to any -- or electronic copies to any of the Committee Members, if they request one.

And then in the last two years we've had these peer-reviewed journal articles. I believe all are published and one is about to be submitted and I provided those to the Committee this morning, reprints.

MEMBER WEINER: Let me just interrupt a moment. Randy has supplied copies of a number of publications and we have -- and we can have CDs made. We have several CDs of the presentation and these will be supplied to the Committee.

MR. CYGAN: Okay, I'm now going to talk about Task 2 and spend about 10 minutes discussing how we're using molecular modeling to help us towards understanding how sorption occurs and one might extrapolate fairly fundamental approach to looking to atoms interacting with other atoms, specific chemical species on the surface of a substrate, such as a mineral, in this case a clay; how we might use that type of fundamental interaction, how we might extrapolate that to looking at Kds. And I'm using Kd in the PA sense, you know, how we could get out a fundamental property, albeit a Kd, but how we can generate those numbers from almost first principles, methods.

And I'm appreciative of the NRC in helping us start a lot of this work. I should also acknowledge that BES funded some of the force field development. That's the fundamental set of interaction parameters.

So let me just describe why this is a difficult task and I've sort of been heading this aspect of the project, so this is one of my pet projects, is to look at how we can use a clay and how we describe atomistically how the components of a clay interact with each other, and then how that clay surface then interacts with the aqueous system and the species in that system.

The problem with clays, and this is sort of a coined term now, a nanocrystalline or nanomaterials, they are almost cryptocrystalline. We don't know the structure of a clay. They don't occur in large crystals that could be on a defractometer and develop a refinement through a refined crystal structure. Clays just don't have that type of ordering, the crystallinity needed to get that type of detailed picture. And often a clay mineralogist will rely on a molecular model, at least the models that we've been developing to have a better feel for how that clay behaves, what its structure is like, how the interlayer varies and just its normal dynamic and structural behavior.

One uncertainty here though is that it's hard to get hydrogen positions, hydroxels. You need to go to sophisticated methods such as like the neutron source up at -- neutron defraction methods like at Los Alamos which we often use. Clays typically are multicomponent systems, have lots of disordering, obviously some vacancies as well. They have very low symmetry, monoclinic or triclinic and I think I already mentioned they have this disordering, especially in the stacking level. So if you have clay layers, they don't stack in a very long-range ordering. They have a lot of disorder here and that's the critical factor and why we don't understand clays with standard techniques.

However, with atomistic methods, we can start to unravel what's going on on the clay structures and behavior. Typically, we require an accurate, empirical energy force field and this is a work that DOE3 BES helped to fund as well. Quantum methods are way too costly. These systems are quite large, many hundreds of atoms. They have large electrostatic fields because of the layered structure and often it's difficult to validate the models.

So here's an equation that pretty much describes atomic interactions, at least the style that we use to do our molecular modeling. It's fairly simple and that's why it's so successful, is that we parameterize interaction parameters, these A, B and Q terms to describe how atom A interacts with atom B or in this case I with J.

If you remember back to chemistry and physics classes, the bulk of interactions are going to be Coulombic in nature. That's simply a 1 over R term, very long-ranging and in this case Qs are the ion charge or partial charge, okay? And then the short-range interactions are described by these A and B terms. One over R to the 12th and 1 over R to the sixth. This is a Vandervals interaction term.

Essentially, you have the electrostatics of like charges interacting. They'll collapse on each other, unless they have a Vandervals term that keeps those two ions apart. Okay?

And what we've done is parameterize all of these terms here by looking at simple oxides, simple hydroxides. We've often done quantum calculations using some high level bases set to look at the structure and as a result of all this effort, we were able to generate a set of force field parameters.

The force field parameters are the key for how we describe atoms interacting with each other. They are analytical expressions that the computer can essentially evaluate for given distance of separation for certain geometry of atoms, okay? So now we take one huge step and we go to a simulation of a solution interacting with the clay.

We've taken lots of baby steps leading up to this. In fact, we've probably taken about six years of baby steps in trying to take force fields for clays into something as complex as an aqueous uranyl solution interacting with a clay.

We've done a lot of validation work on looking at just the standard structure for clays when we do know their structures. They've all been validated with this method. We've done a lot of quantum work as well to go along with this, but we have a lot of confidence that this force field is doing what it's supposed to do. The force field is very sophisticated in that it also allows you to look at vibrational spectra, something that is well beyond the typical molecular modeling approach and this is -- this Clayff has been quite successful.

So here's the simulation cell. Obviously, these are done on clusters or super computers. These are nontrivial calculations. This is an aqueous system of uranyl and sodium and there's some carbonate up here in this aqueous system. Here's our clay substrate. It has an inner layer of sodiums here and there's also an external surface down here. This is a periodic image, periodic boundary conditions, so you could extrapolate this cell in three dimensions. And so part of the calculation requires that we do that.

What we're trying to look at is how often we start to form these uranyls and here's the uranyl here, the central uranium and the two oxygens associated with the uranium and then it's coordinated with carbonates.

What we're trying to do is run a molecular dynamics simulation of this system. We did it for a pryopphyllite substrate, as well as two different montmorillonite substrates. The pryopphyllite was chosen because it has zero charge. Montmorillonite clays have charge developed in the octahedral layer by substitution, very standard soil mineral. Montmorillonite has some variability in its charge, but here's a low charge montmorillonite and a high charge montmorillonite.

Sorption is primarily going to be directed by the charge, electrostatics, okay? So we didn't expect to see much sorption of pryopphyllite. If it does occur on pryopphyllite, it's a very local effect.

We run MD simulations under these conditions and let me just show you what we can get out of these simulations. This is backing up a second here. Typical property structural data we can get from these simulations, obviously, we compare that with the fraction. So this is our validation approach on the right.

We can look at local atomic coordination through simulation with the generate RDFs, the radial distribution function, knowing the local geometry and obviously, I mentioned earlier we could associate that with sorption x-ray spectroscopy, in this case, x-axis, for example.

We could also look at interfacial structure through atomic density profiles and experimentally, we can work with the advanced photon source at Argonne, for example, or Brookhaven and generate a high resolution x-ray scattering work to compare.

And then as I mentioned earlier, we can also get vibrational data with this force field, something called the power spectrum and compare that directly with observed infrared and Raman data.

This is just background on the force field. Clayff is the main emphasis for the clay. Some of the other aqueous species are brought in through some other force fields, just an idea of what the charges might be.

What we did in this particular case, we ran 10 simulations of 1 nanosecond each. That means we took a million time steps. This is a very high level amount of calculation time, taking one million time steps of one phempto second. So we're looking at very detailed time scales. This is well below what is expected for vibration of an Oh, for example.

Here's an example of the RDFs. This essentially is showing you the uranyl carbonate interaction in black. The uranyl water interaction, the other coordination ligands here and then you can get off into the diffuse region. This happens to be the second oxygen on the coordinated carbonate group to the uranyl, this black one there.

We started looking at the aqueous speciation --

MEMBER WEINER: Randy, excuse me. What is your X axis?

MR. CYGAN: Oh, RDF, radial --

MEMBER WEINER: That's the Y axis.

MR. CYGAN: Oh, I'm sorry, the abscissa is R, distance in angstroms.

MEMBER WEINER: Thank you.

MR. CYGAN: Now I'm presenting this detail so you can see the extrapolation now into generating a reaction constant for a sorption. We're going to look at uranyls sorbing on to the clay to get this association. And obviously, you could write a reaction constant for that and convert that to a Kd.

And this is essentially the mechanics of how we go about doing it, essentially flip the cell on its side and we generate an atomic density profile that is the density of a particular atom over the whole simulation time as a function of distance and we try to correlate the actual image with the profile below and you can start to see the sodiums in the inner layer. Here's a sodium peak. There's another sodium peak. These are sort of the aqueous like sodiums and this is the clay. This is the clay. And then all the action that's critical for deriving Kds is out here. Here's the sorb uranium peak that occurs right here. There's two uranyls that are sorbed to this particular surface and then we have a diffuse region where the uranyl concentration changes as we go out into the bulk.

So taking all those simulations, I forgot to mention that we did 10 simulations of a nanosecond each. From that, we could generate a Kd and here I plotted Kd for the montmorillonite, high charged; montmorillonite, low charge and the pryopphyllite as a function of the carbonate concentration. We vary the carbonate concentration in the solution.

Now this is just showing the extreme detailed level that sorption can occur differently on the same mineral, but a mineral having different charges, low charge, this is high charge. Obviously, the Kd, almost by a factor of 10 variation in this single phase. Okay? Comparing that to pryopphyllite, and this is a log scale, you can see that pryopphyllite, as expected, has low sorption represented here.

Now we extended some of the simulations out to a large carbonate region without modifying the uranyl just to get an end limit.

We showing the results as Kds. Obviously, we could generate a surface complexation model on these data. But if we're just generating Kds, this is demonstrating what we wanted, so the point that we got out of all of these simulations is that we form carbonate species out in solution and I think in Jim Davis' introduction we talked about the carbonate complexes that form with uranium and here we are in this force field with this simulation, we're generating the same type of carbonate groups. This is a tryscarbanato uranyl complex that occurs out here.

And we could plot sort of like the species diagrams, we could plot the species as a function of carbonate concentration and then you can see that the uranyl species decreases as carbonate increases and we start to form, even for pryopphyllite, we start to form these carbanato complexes. For the montmorillonite, you can see the uranyl dropping at the sake of forming the uranyl carbonate.

And this is just a summary slide of what we're seeing here, the fact that you have absorption occurring as the clay layer charge increases, going from pryopphyllite to montmorillonite. And then as the concentration of either carbonate or uranyl increases, we start to form these aqueous species. So this is almost a validation approach for our molecular model, seeing that we're on the right track. We can look at exactly at what's happening in the real world in terms of forming carbonate complexes with uranyl, especially if the concentration goes up, these guys are stable in solution and therefore they're going to have major effect on the transport. You're not going to be sorbing uranyl as strongly if you have high carbonate concentrations and therefore you're going to have further transport down into the groundwater stream.

I'm going to move to the next task.

MEMBER WEINER: I think we have some questions.

MEMBER CLARKE: Randy, this may be premature or this may be where you're going, but are you looking at desorption as well?

MR. CYGAN: Yes. These studies are looking at local equilibrium if you will, in some cases that has both sorption and desorption. For the time period of the simulations, you do have these sorption processes, so you're looking at competition from sorption, desorption and ultimately an equilibrium.

MEMBER CLARKE: You can look at the concentration in the water and look at what comes off the clay as well.

MR. CYGAN: We could if we had the confidence in our force field that we would be representing that properly, but we have not done that. We've always looked at full saturated systems.

MEMBER CLARKE: Thanks.

MEMBER WEINER: Anyone else at this point?

MR. CYGAN: All right, well, forgive me for the indulgence here in terms of getting the beginning talk being fairly heavy on the molecular modeling, but I think it demonstrates the build up into all the other aspects.

Now I'm going to presenting work that Louise Criscenti headed with regards to uncertainty analysis and how you look at different sorption modeling and how scaling comes into play and how well this can be used to predict sorption processes.

This is just to demonstrate one of the failings of a Kd approach looking at the activity or concentration of an absorbate, just the ratio of the sorption to the aqueous solution. When you measure a Kd, it's at a very specific composition, a very specific ionic strength, a very specific pH and here's an example of a sorption isotherm that is percent of some radionuclide or some metal. In this case, I believe it's cobalt, percent of sorption as a function of pH. And you can as you increase the pH, you start to sorb more and more of the cobalt. That's because the surfaces of the gypsite are getting more and more negatively charged, as you increase the pH. The surface chemistry is changing. There is more deep protination of the surface, more exposed oxygens with negative charge. The cobalt increases on the surface.

But if you do the same experiment at a different concentration, you could see fairly drastic differences in the percent sorbed, for example. Here, you have one occurring at 50 percent for .01, but if you go to one molar concentration, it's going to be about 85 percent sorb.

So very specific conditions are involved in doing a sorption isothermic experiment. Okay. And you just can't take the Kd and extrapolate it to other environments, different chemistry, different compositions.

Louise has this sort of a conceptual model of what happens when you have a landfill, for example, being leached, contaminates being leached out and going into the ground water system, interacting with various oxides. You see the pH change, concentration changes, obviously, as we go through this chromatograph, if you will.

This essentially fundamentally what's involved in a reactive transport model and how we incorporate sorption into that reactive transport model will be extremely important. Aqueous speciation solubility will come into place and the sorption here is either going to be a Kd or a surface complexation model. And we'll be comparing those.

So what are the uncertainties in a conceptual model? Let's define -- first off, you need to define the system in terms of the expected aqueous speciation and in this case for calcium system with carbonate, carbon dioxide equilobrating with the water. You need the fugacity of the CO_2. Obviously, we form calcites and carbonates within the aqueous system. Calcium species, calcium complexes. We have the possibility of having precipitation of calcite, also the dissolution as well. We can form some ferrihydrite which is a very common sorbing phase. It's coating most quartz feldspar in the ground water system in soil systems. It's the coatings that are critical players.

And then as noted earlier, we have to compare kinetic versus equilibrium models, see if we can incorporate these rate terms and then our emphasis here has been on the absorption model, which one should we use.

In the field, there are some concerns about making these measurements. Jim Davis in the USGS have done a great job, spectacular job, if I may, at the Naturita site, and it's sort of being used as a test bed for applying surface complexation modeling. There they've collected tons of aqueous data. They're looking at certain minerals and Susan is going to discuss some of the characterization studies of the minerals, what specifically are the minerals that are absorbing the contaminants.

I already mentioned ferrihydrite. I mentioned earlier clays being critical players in the sorption. We also need to know the reactive surface area of each of these solids.

That didn't get translated right, but for a surface complexation model, you have several flavors to choose from: semi-empirical models, where you essentially fit parameters to observed data and Jim

Davis will describe for Naturita the use of the generalized composite model. Essentially, it's a matter of taking some soil from the field, doing some bench experiments, looking at some tracers and seeing how they're sorbed and from that you fit something like a surface complexation model to those data and you essentially have the fundamentals of the thermodynamic sorption model.

There's something called the single site model which is pretty standard in a lot of the geochemistry codes. And there are several flavors of these. And I'll talk about those shortly.

And then the more sophisticated models, the multi-site model involves looking at a very specific chemistry of that substrate, of that mineral surface. In other words, do we have a protinated site or do we have a de-protinated site? Do we have a cleavage surface of a mineral that has different groups being exposed, different coordinating ligands? And so the music and CD music model address that issue.

The fundamental question is in how much detail do we have to go to describe the interface where the sorption is occurring? Can we extract acceptable reactions to alchemitries from bulk sorption data?

Do we have to get the particulars of the surface species? Do we have to use spectroscopic or even molecular modeling tools to be able to write the sorption reactions?

Then questions that come up on the surface sites: can we treat all the sites as being some average value that represent all the chemistries occurring at that substrate surface? And then that's for a mineral and then can we use these same average sites to describe a more complex mixture of minerals such as in a soil.

These are pretty fundamental questions and hopefully, so far this morning, I've given you some examples of how complex these systems can be.

We have the Star of David now instead of the electrostatic potential, but this will do.

(Laughter.)

This is electrostatic potential. That's a function of distance from an interface. The constant compacitance model, diffuse layer model and a triple layer model. The surface is to the left. This is a surface and this is going into solution from left to right.

Each of these models has its own level of complexity in describing sorption. As I already mentioned from the molecular modeling approach, the electrostatics are crucial. If you don't know the charge distribution, the electrostatic potential at that interface, you're going to have a very difficult time describing where the cadions and anions are going to go.

So the diffuse layer model, CCN, was like the first attempt to try and describe how the electrostatics change as a function of distance. And here you have two sorption -- thermodynamic parameters plus a capacitance. And the diffuse layer model, you have a different description of it which is two sorption parameters. The more complex, triple layer model actually tries to look at the distribution on the interface and the zero plane. This is where you're looking at protination schemes on the interface. And a beta plane where the sorption occurs, and you try to fit these parameters or try to get those parameters.

MEMBER WEINER: Excuse me, could you give us some idea of the scale of the axis, the scale of that X axis?

MR. CYGAN: Well, on this schematic, deliberately we tried not to, but in practice, you can expect a lot of this action to be occurring in the first maybe within five angstroms of the interface. And some systems, based upon the dielectric of the substrate, this can be quite substantial, maybe up to 10 angstroms or 20 angstroms. So also depends upon the sorbate, what material is sorbing to the service.

MEMBER WEINER: But it is of the order of angstroms or a chance of angstroms?

MR. CYGAN: Yes.

MEMBER WEINER: Thank you.

MR. CYGAN: But trying to describe this type of detail, obviously, is a tough one.

I already showed you a molecular model. This happens to be water on gibbsite and here, in this case, we show that electric double layer to be on the order of about 8 angstroms, I believe, or 10 angstroms here.

It's really looking at this fine structure from the atomic profiles. You can start to see, in this case, here's a water oxygen in red that's fairly well coordinated. Water is a sorbing material. The water molecule sorbs to the surface quite structured and it sets up an electrostatic potential because of the partial charges on the oxygen and the hydrogens. And then you can start to see some structure and as you go into the second part of the double layer where the protons and then second water has occurred.

One thing that we had done and Louise Criscenti headed this particular task, we were looking at what the uncertainties in a surface complexation model, how they're passed along in the calculation. We wanted to look at the fundamental variation in the log Ks, in this case for deprotination and in this case for sorption.

In this reaction, you have let's say gibbsite or clay or something that sorbs, the aluminum compound. We know that in order to sorb a uranyl onto this aluminum compound, we need to first deprotinate the surface or excuse me, to protinate the surface to form ALOH. Now we're going to look at a log K for this reaction here and from the literature, we got a value around 9.7.

We then looked at another log K for the same surface reaction site, but now the formation of the complex, the uranyl complex, given by this reaction here. And here we had a mean value of -2.7. It's a fairly complex system. These aqueous components are aqueous components -- are complexes formed. Again, there's the ubiquitous carbonate uranyl complexes that can form. And what we did, we looked at a smectite, a smectite clay. And the aluminum is an edge site on this particular clay. There's the aluminum. If you cleave the clay surface, you're going to expose the aluminum. The aluminum oxygens will interact with the aqueous system and there's an acid base reaction that occurs. And that's pretty much described by this log K here.

So what we did was ran reactive transport models on this system. We did 100 realizations based upon Latin hydrocube sampling. So we took this mean value for the log K here. Took this mean value for this log K and ran 100 realizations and we plotted the breakthrough curve, at least we monitored the concentration front as a function of distance for two years. And we wanted to see how the variation of these two log Ks would affect this value.

So immediately, we saw that the data broke up into two different groups. Group A, a Group B. The base line is right in the center here. This is actually a Kd model that we used, just for comparison sake. You can see the difference here is enormous in terms of after two years, the distance for the concentration front varies from let's see, around 10 meters in one case, up to about 250 meters in the other case on the two extremes of the log K.

Anyway, we could break down the data into distance as a function of log K of the complex former, the uranyl complex and this is the acid dissociation. And you can see the acid dissociation of log K actually makes this distinction between group A and group B.

I know the Survey has also done work for Naturita in a similar fashion, using some statistical approach to sample of the Log Ks into surface complexation model and I believe Jim Davis will be talking about that at your next chance to review his program.

Louise was concerned in setting up this part of the project, just trying to see how far we can bridge this gap between the field out here and the atomistic level down here. And this is just a standard log plot of the distance versus time and where our simulation methods fit in. Obviously the application is up in this right hand corner, the atomic detail down here. And trying to see how far we can push the information that we gained down into understanding what's going on up there and how we apply surface complexation models.

I think I'll skip this. I just said that.

I'm just repeating here the need for an

internally consistent set of parameters is critical in understanding sorption. To date, a lot of the researchers are relying on the classic, I believe it's Zomback and Morrell. I think it's 1990 or 1991. It's a compilation of sorption parameters that are available for looking at how a variety of different metals will sorb onto ferrihydrite, some iron oxide face and a lot of people rely on those data sets and that's getting pretty dated.

There's a need for a lot more data, a larger number of substrates, so a lot of work is being done and heading in that direction.

MEMBER WEINER: I'd like to stop at this point and entertain questions.

MEMBER HINZE: A simple question to make certain I'm understanding. Should we be concerned about saturation in the sorption and how well can you predict that modeling?

MR. CYGAN: You mean a saturated surface with some species?

MEMBER HINZE: Yes, is that a concern?

MR. CYGAN: It's going to be a concern, but if you have the right mass action laws and you know your sorption densities, it will be handled by the surface complexation model.

Not all these models are capable of doing that, but we know what the loading is. If you get to some of these more complex sorption models, you could examine that. Obviously, for these concentrations, let's say in molecular models, we know we're not at saturation. But if we had enough solute in the solution, we could certainly saturate, as long as we're meeting charge needs to get the sorption to occur.

MEMBER HINZE: If you have enough time too.

MR. CYGAN: And enough time, certainly. But part of the input into all these -- into the diffuse layer model, the triple air model and all that you need, site densities, knowing how many sites are available. You need to know the surface areas.

MEMBER HINZE: How well can that be predicted, for example, if you characterize a site in terms of its mineralogy?

MR. CYGAN: Well, you know, a lot of these are generated by empirical fits. You do the sorption experiments and you'll be able to generate those if you look at titration curves, for example, then the sorption isotherm. You can do it that way. It depends on the quality of those data. And you know certain groups do great work. Other groups do not. So you see a lot of variability in that.

So the molecular models help a little bit in terms of site density, assuming you have equilibrium, but yeah, there's a lot of complications that are involved in that.

MEMBER HINZE: There are modeling procedures for this, but not all of them include that, that's the bottom line.

MR. CYGAN: Right, right.

MEMBER HINZE: Thank you.

MEMBER CLARKE: Allen?

VICE CHAIRMAN CROFF: No questions.

MEMBER WEINER: Jim, I know you have questions.

MEMBER CLARKE: This is a quick one, Randy. As you mentioned, you're working with very complex systems, aqueous systems with different species. Have you done any vapor phase work which might be a little simpler and just to check out your predictions and your agreement with experiments?

MR. CYGAN: With regards to --

MEMBER CLARKE: Something simple with enclave -- maybe not a radionuclide, maybe an organic solvent.

MR. CYGAN: We have done studies on the molecular level with vapor, looking at what happens at the liquid vapor interface and we have a good feel for partitioning there.

We never really pursued it in depth for unique systems that can be validated.

MEMBER CLARKE: It seems like it might be a simpler system. You're looking at a molecular level.

MR. CYGAN: Yes. That's a good bit of validation set of experiments. That's a good idea. That on its own is a very -- it's nontrivial, just what I've demonstrated here. We just have not put our effort into that aspect.

We often rely on how well our molecular models, for example, we have enough experimental spectroscopic data, defraction data to help keep us honest and validate it. So we don't feel that we're pushed in a corner with our models. We think they're robust enough that they're doing a pretty good job, especially with the results I presented on performing the uranyl carbonate species and showing their correct trends.

Some of the other surface complexation models, the more macroscopic type modeling, they do pretty well on some idealized systems, but I don't know of any vapor aspects.

MEMBER CLARKE: It's very interesting stuff.

MEMBER WEINER: I just have a simple question. Have you looked, theoretically, as well as actually, at other complexants than carbonate?

MR. CYGAN: For right now, all of our work has been concentrating on either cesium or uranyl in terms of the modeling, the molecular modeling. So no, we haven't gone beyond those. We could easily introduce them into the molecular model for that type of system.

MEMBER WEINER: Are there any that you think might be particularly interesting in this kind of system?

MR. CYGAN: Take your pick. Carbonates, sulphate systems, anions. I know the NRC Research Office has been very concerned, for example at looking at iodine for example, but we haven't gone that route yet.

MEMBER WEINER: That's for another time. Do any member of staff -- Neil?

MR. COLEMAN: Neil Coleman, ACNW Staff. To use the specific field example in terms of the area available for complexation, at Yucca Mountain, the terminal part of the saturated zone flow system is in valley falaluvia, so you're outside of this realm of fracture flow.

What's your sense of the efficacy of complexation and the volume of material that's available when you also consider matrix diffusion processes which you hadn't been talking about here in that sort of environment?

MR. CYGAN: I don't know. I don't have a good feel for that myself. I think Jim Davis and the Survey people would be better at answering that question.

I think if you saw the -- I don't know if you personally have reviewed the Naturita material, but the Naturita has some aspects of that alluvial fill type basin and gives you a better feel for some of those concerns that come up. I don't know specifically about the matrix diffusion effects though.

MEMBER WEINER: Will Jim be talking about the application to the Naturita site when he talks to us?

MR. CYGAN: Yes. He will give you a lot more of the hydrologic detail and how SCM fits into that model. I just can't answer that. It's not something I'm familiar with right now.

MEMBER WEINER: Anyone else? Soldier on.

MR. CYGAN: Okay. I'm almost done here on my part. The last thing I'm going to mention is trying to implement how one would go about making the decision about using surface complexation models versus a Kd. And part of that is just providing a tool and this tool was generated in response to the NMSS group, trying to have something they could give to the licensees that they could test to a particular site, be it a containment facility at a power plant or some tailings at a mine, trying to figure out when is a Kd appropriate, when is an SCM appropriate.

And so Geoquimico, Glen Hammond is one who generated the -- did all the programming for this particular tool. He wanted to keep a Southwest flavor to it and so he used Geoquimico as the name for the software tool.

But anyway, it essentially take surface complexation models to diffuse layer model and implements it into a nice easy-to-use, user-friendly, graphical-base interface and I don't want to read off all the slides here, but there is concern about trying to make it user friendly and using up-to-date codes.

Actually, it's written in C++ and in Java. And so it's fairly easy to convert to other platforms.

There was some concern about a lot of the active codes that are available now, is that it's very difficult to input the data and also to have post-processing, obviously not very user friendly. And the decision was here trying to get something that was fairly easy to use, something that's state-of-the-art in terms of conceptual modeling for surface complexation models, also, with the support of the NRC, something that the users, the regulators can provide to their licensees.

It also allows a basis for comparing sorption models, trying to figure out the validity of one versus the other. I think a lot of this I'm repeating with regards to the licensees. User friendly. And the last one here is something that we were pushing, trying to make it web-based. So it would be fairly easy to send out to the licensees, also fairly easy to maintain and that's why it has some Java component.

Less steep of a learning curve. I already mentioned the input is less complicated. Let's see, faster turnaround, more defensible results. Allows you to compare the different models, sophisticated models. Let's see, updates available, fairly easy to deploy updates. It's independent of a platform and the GUI. So forgive me for just reading off the slides here, but in this case I could describe much better.

This is a standard input and I won't mention the code, but this is what you typically have to deal with surface complexation models, okay? That's the problem. You have to be an expert. These are typically academic codes, very user-specific generated codes and not often codes you just pass out to the general public. There are a couple out there, some commercial codes now that are a little bit easier, but there's some licensing issues with those.

Object-oriented, platform independent. The GUI I already talked about.

There are some disadvantages. There's a question about speed and then also the legacy issue, do people really want to convert over to yet again another code? And with what Glen has generated, we have a nice little package here. This is essentially the interface for Geoquimico, fairly straight forward in terms of adding your components. You obviously are not going to be able to read these up on the screen, nor probably in your handout, but essentially, you have pull downs for all of your basis, for all the species that you want to look at. You also could put in your sorbate information, the species here. This example happens to be for lead.

We chose in debugging this code a lead system that had been published and a lot of work had been done in validating that model, so we use that as our comparison, our standard. Right now, Glen -- well not actually -- Glen was working on trying to generate some uranyl scenarios that are much more specific for radionuclide studies.

He uses a 1D transport, finite volume, formulation for the fluid flow; aqueous complexation, sorption, given one of these three possibilities. Surface complexation, a Kd and even an ion exchange. There are a series of preconfigured schemes that can be tested, just for examples. And then in the last couple of months, this summer, he's introduced uncertainty analysis, trying to look at these parameters and how they might vary. So he included some Latin hypercube sampling. He has some log normal distributions for the input parameters.

And here's an example. This is a breakthrough curve for lead. I believe it's lead sorption onto a ferrihydrite using a Zomback Morrell database. Essentially, this is a log of the concentration as the function of time and he gives a direct comparison of what happens with a simple Kd model versus this diffuse layer model, the surface complexation model in terms of the long tail that goes over, in this case, 2,000 years, still above the MCL value, whereas the Kd model and this is a very good example, at least for the case of lead, the variation and the major significant difference between the simple versus the more generalized model.

MEMBER WEINER: Do you have -- before you leave that slide, do you have any comparison with actual measurements to see which one is closer?

MR. CYGAN: Nobody has been working on this. I don't mean -- nobody has been working on this for 2,000 years, so -- but that's one of the issues we have here. I don't know the experimental data associated with this particular problem. So I don't have an answer for that. I don't mean to be glib about it. But yeah, that would be the critical thing aid make that comparison.

The best test for this is to do a Coloumb experiment and start to compare one versus the other and I'll actually address that at the very end.

For this code development, there's a wish to continue on with regards to having more uranium-based scenarios or other radionuclides. There's a need to improve the plotting capabilities, vary the distributions in something more non-standard for the uncertainty analysis and modifying some of the sorption species and some of the ability to save the scenario, save in load features.

I think I will stop here and I will pass it along to Susan, unless I can answer any questions now.

MEMBER WEINER: Are there questions?

CHAIRMAN RYAN: Why did you pick uranium instead of plutonium or --

MR. CYGAN: The uranium was emphasized primarily because of Naturita. We were trying to work with our collaborators at the Survey. Susan will emphasize that when she presents the characterization study next. But the Survey was trying to demonstrate surface complexation modeling, its benefits, specifically for the Naturita site.

CHAIRMAN RYAN: So the uranium was there and you picked it for that reason?

MR. CYGAN: Yes. Naturita is an UMTRA site and it has the contaminated ground waters there. Even though it's been cleared off the top soils.

CHAIRMAN RYAN: The reason I ask is it would be unusual for uranium to crop up at the top of the hit parade for PA.

MR. CYGAN: Right, understanding that. Everything we've been working on has been trying to coordinate with that, but I understand.

CHAIRMAN RYAN: Gotcha.

MR. OTT: I'm going to add a little perspective right here. About six or eight years ago, you remember, Randy, we had a little workshop out in Menlo Park that was associated with the end of one of the Alligator River programs.

We were raising a lot of questions at that time, based on a lot of resources being spent on sorption work and were we ever going to get anywhere because we still weren't being able to use these things in PA.

And I asked the question to the group if there was anyplace that would actually apply this stuff and Jim Davis came back and said well, based on the work they'd done at Alligator River and they had been studying Alligator River for almost 10 years at the time, he said they thought they had enough information on uranium to actually do a field demonstration site someplace in the U.S.

So the next thing we did was challenge USGS with a demonstration project to go out and find a fairly chemically complex uranium recovery site where uranium was the species they were interested in. So it was a fact that we had developed enough information on uranium that drove us to continue using that as the way of demonstrating the technology.

CHAIRMAN RYAN: No, I fully appreciate that, Bill, thanks, but again, it's a low priority in the PA world.

MR. OTT: It probably dominates a lot of systems like low-level waste sites where they put a lot of depleted uranium. I mean the chemistry of the uranium is probably fairly important.

CHAIRMAN RYAN: It's a toss up. But I understand your point.

MEMBER WEINER: Allen, I have a question. Why Latin hypercube sampling and not Montecarlo sampling?

MR. CYGAN: For Geoquimico?

MEMBER WEINER: Yes.

MR. CYGAN: I can't answer that. WE've been using -- Montecarlo sampling has been used before for these type of comparisons for uncertainty. I believe he actually has an option to get both in there. I don't know why that was the one that was chosen initially.

MEMBER WEINER: Normally, you use Latin hypercube sampling when the number of samplings you can do is fairly limited and you want to get the whole curve. But we found that if you have enough samples, that's not a problem and you don't over emphasize any section.

MR. CYGAN: Well, for the reactor transport modeling from Louise's effort, that comparison with the sample A and sample -- or Group A and Group B, that was obviously a Latin hypercube sampling approach that's needed.

MEMBER WEINER: Yes.

MR. CYGAN: The geochimico probably is less constrained and certainly Montecarlo may be a better option. I just know he has several options for the uncertainty analysis. But I don't know why one specifically was chosen over the other first.

MEMBER WEINER: Thank you. Neil, you had a question? Latif?

MR. HAMDAN: Randy, good presentation, thank you.

The question I have from the standpoint of that this is your maker, you give him these two options. The Kd based approach and surface composition model and leaves the impression who does that. Are these the only two options actually available that state, for example, if a particular site, just one site, is it an option, for example, if uncertainties are so large that the envelope will do or no nothing maybe is equally good?

MR. CYGAN: An excellent question. I think to answer that is that you really want to have something that's defensible when you have a PA code. And I think the point here is that you're relying on the state-of-the-art thermodynamics to describe the simple sorption process or the not to simple sorption process, if you will and taking the short cut with the Kd is going to be introducing substantial amount of additional error that cannot be accounted for. Essentially, you're not describing what's happening, especially if you're trying to push PA codes to 10,000 years. We know that the solution concentration is going to change here on its strength pH. Dissolution precipitation so on and so on.

A Kd is a very specific sort of an ad hoc, that's my term, way to describe partitioning and it's only that, where as the SCM has a lot of history, a lot of theory, a lot of modeling basis that describes exactly how activities or concentrations will change in a complex system.

So to generalize it with an SCM is critical and defendable, whereas a Kd it's more of a stab in the dark if you will.

Now there are some systems that are simple, simplified that you can get away with a Kd, as long as you have the constraints of words of isothermal, iso -- the pH doesn't vary, ionic strength is invariant and that sort of thing. And it might be applicable. But it would be hard pressed to defend that when you have to start defending the transport behavior at 10,000 years down the road.

So I think you do have the choice, but you're playing sort of on the -- on the uncertain side.

MR. HAMDAN: I'd like to see and this is the -- I think about that. Is a third choice. Things are those complex, so far in the future. Let's say 10,000 years. Can you model -- can you, for example, just as an example, you can say in this case I can model for 500 years or a thousand years, end of story, the farthest I will go and that happens between now and in 50 years somebody will -- the chronology will improve or the modeling will improve -- why isn't there a third choice? We are presented with choices that are the researchers are working with and there's no third choice, it seems to me, all the time. There's no third choice.

MR. CYGAN: Well, actually, there is a third choice and that's why Jim Davis' presentation is somewhat critical because Jim has actually introduced the generalized composite model. It's something that we allude to in our work, but really the generalized composite model is being applied to the Naturita site as a way to get beyond the complexity of a surface complexation model that has perhaps too many parameters, too many new parameters that might lead to additional uncertainty. And in a generalized composite model I alluded to is essentially where you do some field testing, lab bench experiments, collecting field samples, do the lab bench experiments and then fit those date to try to get new parameters for new complexation model.

So it's sort of like an in-between approach. It's somewhat semi-empirical.

So in a sense, that's probably a good option, a viable option, at least for the Naturita uranium issue and perhaps for some of these other issues with more critical PA type radioisotopes.

MEMBER WEINER: John?

MR. FLACK: John Flack, ACNW staff. I have a question with respect to where we have just been over in West Valley and I guess the question, of course, is you know there's a strontium plume there that they are collecting information on and whether or not that information provides an opportunity for using that to validate your model. So have you thought about that? Or has research thought about that at all?

MR. CYGAN: Actually, yes, we have talked in the last year and a half about considering West Valley as an optimum site for us and that remains to be seen if we're going to pursue that. But we talked with people who have had some experience at West Valley. The strontium plumes have been described and there's a lot of complications involved in understanding that.

I don't have an answer as to it's appropriate or not in terms of applying some of these until we have a better chance to analyze the available right now. I know there's some difficulty in terms of DOE and EPA and the NRC in trying to get access to the site, to this type of analysis. So but yeah, that was being considered, but our contract was coming to an end and we sort of stopped pursing that.

I don't know, Bill, you want to make additional comment or not on what's going -- okay.

MR. FLACK: But there's no reason not consider that information if it's available.

MR. CYGAN: Frankly, I'm surprised why they haven't done it already. I think it's been mostly the sampling and trying to characterize the plumes, but not much work has gone into getting more sophisticated groundwater flow models, reactive transport type models into it.

It's a good challenge, I'd say.

MEMBER WEINER: Actually, I have a somewhat similar question about the Hanford site, because there you have a number of radionuclides in various stages of absorption and dissolution flow on subsurface level and they've been doing it for 50 years. So have you look at that site at all?

MR. CYGAN: Colleagues and collaborators have been working up at Hanford and looking at the leaky tanks and so I know some work is done. I don't know the particulars of it and I don't know how sophisticated the surface complexation models. I could provide some names for you to contact, if you want to get more information, but I don't know them first hand.

MEMBER WEINER: I was thinking for more to you to use this as a validation and not just the leaky tanks, but from the radionuclides from the French drains which were -- don't directly enter the subsurface.

MR. CYGAN: That's obviously one of the applications that can be done. We just have not pursued that.

MEMBER WEINER: Any further questions or comments? Hearing none, let's continue.

I'll speaker while they're transferring is Susan Altman from Sandia Labs.

MS. ALTMAN: Thank you. I'm Susan Altman. I 'm actually an experimental hydrogeologist working with Randy's team and I'm going to talking about some characterization work we did on soil aggregate samples,mostly from the UMTRA site, although I have one slide on some samples we recently analyzed on the Cape Code site. So this is getting at the data to provide the model.

So the purpose of this, well, let me just talk quickly what we did. I've divided this talk into two sections, destruction characterization using microanalytical techniques and I'll go into more details and explain the acronyms later. And also, nondestructive methods using microtomography. And we're looking at two things. One is examining the association of uranium with different uranium absorption with different mineral phases and also with the tomography work, we use cesium as a proxy for uranium.

And then the second part is to characterize the iron-bearing minerals. And I put this beyond XRD as a reminder, you know, generally use XRD refraction to characterize the samples. But we found in a few samples is the iron-bearing content is such a small volume that when you do this you have an overwhelming signal from the cords of feldspar and you're not going to see the iron. So that's why we had to get into the more high fidelity microanalytic techniques.

This is the same point we're going to be saying over and over again of why are we doing this. Traditional approach is using the bulk distribution Kd values. You get an average effect. Leads, in general, to overestimation of plume, underestimation of difficulty of removing contaminants and so what we're trying to do is provide data that feed into an alternative to the Kd approach where we're going to be able to look at variation of absorptive properties which is why we need to look at different --figure out the different mineral phases, account for reversibility, irreversibility, lead to more accurate model. So bottom line is we need more detailed information on the substrate.

Oops. Okay. As we said, we're looking at a number of techniques and the main idea, one of the main ideas I hope you get out of this is that each technique has pros and cons to different scales that you were looking at the samples, different detection limits, but by putting them all together with this multi-scale approach, you get a complementary story.

And again, we divided it into two studies, the microbeam studies, Carlos Jove Colon headed this study. The pros of this, you're going to get, identify the important minerals and absorbing phases, be able to see the composition of the samples and really see association of iron and uranium on the samples.

The tomography work, it's a little larger scale, so you can examine an entire aggregate sample. You can estimate mass fraction ions, so you're not going to get the exact mineralogy, but you can see how much iron there is in there. And with knowledge in mineralogy from the microbeam studies, you can get some sense of the mass fraction of the different minerals.

Again, it's nondestructive and potentially it can be coupled with transport experiments so that's the advantage of the nondestructive. You could see what's going on with these experiments.

Okay, so first let me go into the microanalytical techniques. Here, I'm just going to describe the techniques, as I said, Carlos Jove Colon headed up this study. There's a NUREG report in review and press describing this work. And there are five different techniques that were used: scanning electron microscopy, energy dispersive spectrometry. Oh, I should say also, the USGS, Jim Davis provided the samples for us, did some of the preparation of the samples beforehand..

There were generally two types of samples that were studied. Again, these are from the UMTRA site. One was taking down gradient contaminated with uranium and that we call the untreated composite samples. So it's untreated, contaminated sample. The other was an up gradient uncontaminated sample and what they did was they removed the carbonates just to simplify, as Randy talked about the association of the carbonates in the uranium makes things more complicated. And we were interested more at looking at the ion phases, association of the uranium with the ion phases. So they removed the carbonates and then they added uranium. So they -- it was a much more controlled sample.

SEM work, we looked at the untreated samples. This was performed at Sandia and each of these -- I have a list of names of people who worked on this. The secondary ion mass spectrometry -- and again, you'll see, I'll have a slide for each of these methods. Again, it was untreated samples. They were put in epoxy mounts and polished and this was performed at Arizona State University. The high resolution TEM, there -- it was both the untreated and the carbonate pretreated samples. There were some preparation of the samples prior to looking at them. This was done at the University of New Mexico.

The micro-synchrotron x-ray fluorescence was done on carbonate-free samples at Brookhaven National Labs, along with the MXA and again, it was the carbonate-free samples.

So now you can see the results. This is the SEM work. The top row is one sample. The bottom row is another sample. I apologize, the color coding is completely inconsistent so it's a little confusing. The scale, this is a 20 micron bar. This is a 30 micron bar on the bottom sample. And again, the inconsistency -- this is silica, but it's green here, red here. Aluminum for both. Potassium -- I thinking this had changes, but I switched my version on the airplane. So this is the old version.

Okay, so potassium here and here, iron and aluminum in this one and aluminum and silica in this sample.

So the main thing you note is we've got a quartz substrate, high silica. We've got aluminum and potassium coatings along the edge. The coatings are on the range of 10 to 15 microns thick. We are seeing iron in the sample and in some cases, it's associated with the aluminum and other cases it's free standing, so there are probably some iron hydroxy coatings here.

This is actually unusual. It's a highly weathered sample with a quartz substrate. You can see high aluminum so there are sort of clays acting as the glue holding the coarse grains together. Here you see the two together and there's some potassium in there. And uranium was below the detection limit, so we weren't able to see uranium with this method. that

Okay, secondary ion mass spectrometry.

Again, we have two samples on each row, looking at different elements. For each, we've got a quartz substrate for both samples. This analysis was a little harder to interpret, but you can see there's clearly aluminum, potassium, so we've got aluminum silicate clays in these samples here, here.

There's no clear evidence of uranium associated with any phases, although there is some hint of it. Oh, I should say, the red dots here are the uranium overlaying on the different phases for this upper sample.

So in the upper sample, you can see clearly some uranium on the aluminum, so you guess there's some association with the clays. In this sample, here's the uranium and the carbonates are similar, so it looks like there's some association there. But again, we're very close now to the detection limits so it's hard to be real confident with our interpretations.

And we're seeing that the coatings are about 10 microns thick, so that's consistent with the SEM.

Okay, the TEM work. I've got the main points --

CHAIRMAN RYAN: Can I ask a quick

question?

MS. ALTMAN: Sure, please interrupt. The previous slide?

CHAIRMAN RYAN: If you could back up, that would be great. I'm a little -- I'm just listening to what you're saying because this is clearly not an area where I have any expertise, but you make an interpretation and then you say you're at the detection limit, so it's hard to make an interpretation.

Which one do I believe?

MS. ALTMAN: I say you believe my interpretation with a grain of salt. If we had other data contradicting it and we had more confidence --

CHAIRMAN RYAN: Can you turn that grain of salt into a confidence interval or something I can get my teeth into from --

MS. ALTMAN: In putting it in with the other analysis, you could -- you know, we have clear -- you'll see later we have clear association of uranium with iron, so you'll be confident of that. And I'm trying to think of the other samples that we saw, an association of uranium and clays. I would say I would want supporting evidence, if I was going aid publish this, or I would redo this. Randy has been telling me that this method is actually -- improve the detection limit a lot, so you would redo the samples and do it.

So I would say if you have supporting evidence, then I'd be more confident. You'd definitely see it, but you know, if you have the detection limit, there's a lot of noise in our data.

CHAIRMAN RYAN: I understand what a detection limit is. I'm just trying to get an analytical handle on it, rather than a qualitative description of it.

MS. ALTMAN: All I can say is give you a qualitative description, given sort of that we're at the detection limit, but I mean when we put the whole story together, you're going to see a clear association of uranium with iron-bearing minerals, be it clay.

CHAIRMAN RYAN: Let me try once more.

MS. ALTMAN: Okay.

CHAIRMAN RYAN: What are you detecting exactly?

MS. ALTMAN: What are you detecting?

CHAIRMAN RYAN: You say there's a detection limit, what does that mean? It's going to show up in color on this photograph or they're making counts per second? What are we doing?

MS. ALTMAN: Do you want to go into more detail?

MR. CYGAN: This is Randy Cygan at Sandia.

CHAIRMAN RYAN: Thank you, Randy.

MR. CYGAN: What we were doing was essentially pushing a technique to see if we have the ability, the sensitivity to get uranium associations for these soil phases. We have had some experience using secondary ion mass spectrometry to do that, but never for uranium. And you have to tweak and optimize the SIMS instrument to enhance the uranium signal. You can modify the detectors and that's what we did on this particular set up at Arizona State. Rick Hervick was helping us on this approach.

And we all had our doubts that we were going to get the signal needed and you're talking counts per second for a scan across the sample. You're rastering a primary beam across the surface of your sample and you're trying to generate counts for some convenient count period while you raster this beam. So you're talking fractions of a second.

CHAIRMAN RYAN: So now we're in an area I understand. We have counts per second and there's some background and there's some net signal and calculated uncertainty. Have you got those kind of insights to share with us?

MR. CYGAN: We did not pursue any concrete absolute uncertainty because of the poor reproducibility of this particular detection set up.

CHAIRMAN RYAN: So my question then and I don't mean to be critical, my question is why do I believe this thing? If I can't get my arms around uncertainty in the measurement, what do I do with it?

MR. CYGAN: I think Susan's presentation really emphasizes that this is sort of a qualitative first attack, preliminary scoping experiment to see can the technique even be used to detect uranium.

CHAIRMAN RYAN: Fair enough.

MR. CYGAN: And that's as far as we pushed it, but since then I've talked to Rick Hervick, this was done about two or three years ago. Since then we've modified -- well, Rick has modified the instrument dramatically and I don't think this would be a problem any more.

CHAIRMAN RYAN: Fair enough. but again, I think the proof is in the pudding of a rigorous statistical analysis, you know, I have background, I have background plus sample. I met the subtraction of background and I've used statistics on the net result to see if that's an interpretable value or if 30 percent of time I'm making it up or three sigma, whatever you want to use. But without that, again, we're delving into new territory and try to push a technique and I very much appreciate that, but I just wanted to get clear about it, so thanks.

MS. ALTMAN: Back to the TEM. The points we want to make are in the red squares. One is -- oh, and I should note here, previous slide was sort of a scale bar of 30 microns. We're now in the nano meter scale, so there's 10 nano meters, 9 nano meters. This one is at 100 nano meters. So we've gone down an order or almost three orders of magnitude in some cases.

But now we'll be able to see the layered illite, smectite as a dominant phase in the samples. This is another example of the layered illite smectite here and this is just a different orientation where you don't see the layering.

We see close codes of the iron oxyhydroxides of the clay. Here's a good -- this is clay again. Oh, I said the illite smectite was a dominant phase. Kaolinite was also observed within the samples, so there are some other clays in there too, but this is the dominating phase.

And so close co-existence of iron oxyhydroxide in clay and also different iron oxyhydroxides, goethite and ferrihydrite and here you see goethite and ferrihydrite together. Again, goethite, goethite and ferrihydrite. So we go down an order of magnitude and we have more evidence for the different mineral phases.

And finally, the synchrotron work with the x-ray fluorescence. Now we're talking about this is a scale bar of approximately a millimeter. Here's the optical image of the sample at approximately the same scale. This the uranium-treated carbonate free sample and you're looking at iron and uranium and you see a clear association of the uranium peaks with the iron peaks too.

In the other technique, we ran two standards. The blue and the red were different standards and the three ones are sample and you can see the peak here of the green matches with the hexavalent uranium sample which is what was added to the sample, so it's not a surprise what we see there. There isn't any change in the state of the sample.

So again, the main is that we're seeing the iron oxyhydroxides as the same for the uranium.

CHAIRMAN RYAN: Let me just follow up.

That's the normalized counts, I guess is what the Y axis is. What are the arrow bars on that?

MS. ALTMAN: Can you respond to that, Randy?

CHAIRMAN RYAN: The reason I ask is you've concluded it's hexavalant based on it matching the green, but I asked the question is it actually in between the blue and the red or do the arrow bars overlap enough the way you can't statistically distinguish one from the other using a T test or whatever test you want. That's the risk. And again you may be able to do that. I'm just saying that's -- you're making a conclusion, yet, I don't see how you can get there without some more detailed statistical analysis.

MR. CYGAN: Randy Cygan, Sandia. I don't know what the arrow bars are on this. I'd have to talk to our collaborators on how that was set up. But I think the main point here is that you're really looking in the shift in EV from one peak to the next and I think clearly you can discriminate one valent state from the other, based upon some fraction of an EV. I don't know exactly what the uncertainties are, but if there's enough confidence that it is the one state versus the other, but I agree, we don't clearly state what those uncertainties are.

CHAIRMAN RYAN: Again, there are things like the instrument uncertainty. That's clearly one part.

MR. CYGAN: Right.

CHAIRMAN RYAN: And then there's the same uncertainty and the prep uncertainty and background and all the rest and until you do a system uncertainty, I struggle with how do I interpret the difference between two curves that are near each other and those kind of scales.

MS. ALTMAN: And finally, let me just summarize microanalytic techniques. Four techniques, two different samples. The main you see the presence of iron-rich aluminum silicate clays. The iron-rich base is present as a small scattering particles in the clay layer. You see presence of uranium in the aluminum silicate clay layer. Due to limitations of the technique, it's hard to see a clear association between iron and uranium. The clays are dominantly in mixed layers like smectites. There's a large population of iron oxyhydroxides. The iron bearing layers are highly heterogeneous and this is just -- we got ferrihydrite and goethite which comes in with the next study. And finally, a close association of uranium with iron.

So let me open the floor for questions before I go into the tomography work.

MEMBER WEINER: So this is just a comparison of your techniques to see what you can do with them?

MS. ALTMAN: Yes, I mean part of it was, you know, they did the XRD work and they weren't able to see the iron. So then it became okay, let's look at a suite of these techniques and see what we can learn from them was the purpose of it.

MEMBER WEINER: Any of the staff have any questions at this point? It's been suggested that we take a 15-minute break because you guys have been going on for quite a while. So we'll reconvene at a quarter to 11.

(Off the record.)

MEMBER WEINER: On the record. Susan, you're talking about the Cape Cod work.

MS. ALTMAN: Okay. So now I'm going to move onto the microtomography work which I led. So I'm awful familiar with this work. This was conducted at that Advanced Photon Source at Argonne National Labs. This slide is attempting to show the whole schematic. This is the hutch where we collected the data that comes out here.

There are some crystals that control. By the angle, you can control the energy. The sample is just a simple aggregate sample, a millimeter or less in diameter epoxies onto a toothpick. So it goes through the sample, through a scintillator which converts the x-rays into visible light, reflected off a mirror and upward into the CCD camera.

So the idea is you take an image of the sample and you rotate the sample a little bit. Take another image. Rotate it a little bit, etc. So you've gone out through 180 degrees. What the images are is how many x-rays are transmitted through the sample and that's going to be dependent upon the composition of the sample.

This is where the tomography comes in. They take the series of images and can put them together and you get a 3-D image of the sample and the interior of the sample without actually having to take the sample apart. So what you're actually measuring is the source intensity over the intensity that comes through the sample and that's a function of the thickness of the sample and what we call the linear sorption coefficient. So the output of the tomography is the linear sorption coefficient for each voxel in the sample.

This is an example of slice of a 3-D image. Again, these are 3-D images but it's easier to show a slice and it actually doesn't transmit very well. But you can easily qualitatively distinguish the different regions within the sample. So we have core screens here. You might want to look at your handout. It's a little clearer.

We have this intergranular material which is more absorbing. So darker is more absorbing to the x-rays and there clearly appears to be two different zones of granular material. So one we call the high iron and the more normal background for granular material. You can also clearly see the epoxy surrounding the sample.

The voxel size is approximately 4 microns on the side and you'll notice this tree-ring structure. That has to do with the tomographic reconstruction and its used more than the data along with other sources or norms and again our scale bars, we're talking about a half a millimeter here.

CHAIRMAN RYAN: How big is the beam compared to the sample?

MS. ALTMAN: How big is the beam? You actually have control of the beam because you have shutters. So the beam, we keep it as small as possible to make sure we complete the sample. So it's in the order of maybe 3 millimeters high and --

CHAIRMAN RYAN: It's bigger than the sample?

MS. ALTMAN: Oh, yes. And then it can be much bigger but then you shutter it down just to control it.

CHAIRMAN RYAN: I'm asking real specific questions. Is the beam bigger than the sample or not?

MS. ALTMAN: Yes.

CHAIRMAN RYAN: Okay. If you have that situation, don't you have built up from scattered radiation coming back into your sample and so forth?

MS. ALTMAN: You do have some scattered x-rays that come. There are some things, they call them ringers, where in the reconstruction process they can remove it. It is also a source of noise.

CHAIRMAN RYAN: But you calculated this I/I0. It actually should be equal to a build-up factor which is also a function of the relaxation life UX.

MS. ALTMAN: Okay. You're getting a little beyond what I know. But what I can say is that in doing the reconstruction they have this background factor, the dark fill, that they correct for which may be accounted for that.

CHAIRMAN RYAN: That's not reflected in your equation.

MS. ALTMAN: This is a theoretical equation.

CHAIRMAN RYAN: Oh, no. It's a real equation. It works like a charm.

MS. ALTMAN: Yes.

CHAIRMAN RYAN: The reason that I'm asking is --

MS. ALTMAN: -- details of the reconstruction and what exactly is it.

CHAIRMAN RYAN: There's a question with narrow beam and wide beam geometry.

MS. ALTMAN: Okay.

CHAIRMAN RYAN: If you have narrow beam geometry and you're trying to measure it with a detector, you're not going to get scatter from bigger beams back into the detector that didn't interact and give you a false positive signal. Whereas broad beam geometry you have to correct for this built-up. So I'm just wondering which circumstance you had?

MS. ALTMAN: And I can't answer that. I don't have the answer to that question.

CHAIRMAN RYAN: Okay. Fair enough.

MS. ALTMAN: It's bigger. It's not a lot bigger. And I don't know where the cutoff is.

CHAIRMAN RYAN: If it's bigger at all, built-up is an issue.

MS. ALTMAN: Okay. So I don't if the dark field -- What they do is every so many images, every 50 images, they have the beam go off and take an image on nothing and they use that as a noise correction. I don't know if that accounts for that or not.

CHAIRMAN RYAN: No.

MS. ALTMAN: Okay. So in the previous slide I showed you this is qualitative information you can get from the data. Now we talk about more quantitative information. So what we did is just make note of the values of the voxels of the linear sorption coefficient of all the voxels in the sample and we get a histogram which is the heavy dark line.

So what I did is I best fit the black line using different means of standard deviations. The blue line shows the air. The green shows quartz. The red shows the intergranular, the more dominant material and this is a blow-up of this slide. So we have here again the intergranular material and then the high iron. So we have the high intergranular material. It's a small volume.

With that, I have a mean and a standard deviation linear sorption coefficient for each region within the sample. And you can see distinct regions clearly. Then you also see -- Sorry.

CHAIRMAN RYAN: What's the standard deviation? I don't see that.

MS. ALTMAN: It's defined as the Gaussian Distribution.

CHAIRMAN RYAN: So it's not an error bar in particular.

MS. ALTMAN: You'll see that later. I'm just showing the Gaussian Distribution which is defined by a mean and standard deviation. If you subtract that from the range, you get these dotted black lines which are either mixed voxels, so you have some voxels that have more than one substance in it, or it could be due to x-ray refraction too or in this case, it's probably some epoxy.

Here you can see -- I should say also along with our aggregate samples that we got from the UMTRA site we took some minerals of known composition and imaged those and measured the mean and standard deviation for those. So that's what this plot is showing is the mean and the error bars are one standard deviation.

The mass sorption coefficient is just a linear sorption coefficient divided by the density of the sample. Theoretically, there should be a pretty linear relationship between the mass fraction iron and the mass sorption coefficient. We're seeing that at the lower ranges because you have other minerals.

The iron's really going to dominate the sorption of the x-rays at lower ranges. When there's less iron other minerals you'll see. So you get off the regression a little bit. But we defined a regression between mass fraction iron and mass sorption coefficient.

What we want to know is how much iron is in the sample or at each region? How much clay and how much iron (oxy)hydroxides and this is where the previous work fits in because they were able to provide us with these are different minerals, these are the compositions of the minerals. So we were able to use that as background and we just set up a system, the four equations, the four unknowns, pretty simple equations just looking at the mass fractions and the relationship between mass sorption coefficient and linear sorption coefficient to solve for these unknowns using this regression.

This is the data input. The ferrihydrite versus gurtite (PH), they're going to have a similar amount of x-ray sorption. We won't be able to distinguish them. So what we did is just bounded values and said we have a mean fraction iron based on the stoichiometries of this between this and this and the same for clays. From the work from Carlos Ovacologne (PH), we were able to have a range of what the stoichiometries were and then able to give a range of the fraction of iron in the clays.

This is the background data that we put into our system equations. Then we come out with either mass fraction iron or mass fraction iron (oxy)hydroxide for the different samples.

The blue and the red is we collected data at two different energies. The lower the energy the higher the quality of the data, the less noise there's going to be. But unfortunately at the lower energy we weren't able to get enough transmission through some samples. So we had to redo it at a higher energy. Actually for this high iron portions, I trust the 26 keV data there.

You're always looking for ranges. We have a range of mass fraction iron given sort of the uncertainty in some of the parameters. I didn't account for the standard deviations which should be there to a certain extent. But we have a range of mass fraction irons and mass fraction iron (oxy)hydroxides if you subtract. We assumed it's just clay or (oxy)hydroxide. So you subtract one from the other. If you subtract one from this value, you would get the mass fraction clay. We're talking values around 30, 35, percent in the high iron dominated by the (oxy)hydroxide.

For most of the samples, again this is one sample here and three other samples. We're talking 20 to 35 percent iron (oxy)hydroxide and about 20, a little higher than 20, percent iron in the sample. So we're hoping this can be input data into the models and it's a simple way to collect a fair amount of data without having to do a lot of sample preparation.

The second thing we were interested in is looking at the association of cesium with intergranular material. We could see that. We used cesium as our tracer. It's highly soluble in water. It's cad ion like uranium and it's highly absorbing to x-rays.

So what we did is we took the samples. We soaked it in a cesium chloride solution. Then we rinsed the sample for a number of rinsing until we didn't see an cesium or chloride in the rinse water and then we imaged it. Now this slide here shows the linear sorption coefficient versus energy.

If you look at quartz, it just decreases with time and the same with iron. But with cesium, you have this sorption edge. At a specific energy, all of a sudden there's a jump in linear sorption coefficient. What we do is we take an image above the sorption edge and below the sorption edge and by subtracting the two, we hope we only see the cesium because with iron, there's not going to be much difference in the sorption between the two.

So this is the image above the sorption edge and below the sorption edge and this is a different image which again is not transmitting very well. You can see a little cesium up here associated with this high iron. There's also some around here. If you look at your handouts, you'll be able to see it better. Unfortunately, we think we had some epoxy in the way of the sample down here. So we didn't see much cesium sorption down here. But we were pretty excited. We got to see the cesium in this sample.

Finally, we just in August got some data on the Cape Cod sample. These are samples the USGS has been working with. It's a well characterized site and we wanted to test this technique with a different sample. What's interesting with this sample is that it seems to be, these are really preliminary results, much more heterogenous than in that of other samples.

We have mass fraction iron ranging from about 20 to 40 percent and actually there was another sample I'm not showing here where it went up to greater than 50 percent iron.

From the literature, these are sort of the potential minerals that could be in the samples that are consistent with the readings we're getting. Also again if you look at the cesium, this is our difference image. We're seeing a lot of cesium sorption. We were a little bit more careful with our epoxy this time. You can't see it here but this yellow circle, there's clearly quartz and our measurement for the linear sorption coefficient is consistent with the theoretical value.

Then there's another reason, slightly more absorbing than another mineral. What's interesting is you see some cesium sorption at that boundary between the quartz and the other mineral. The rest of the cesium you see associated with the intergranular high iron materials.

What I'd love to be able to do is we need to finish the evaluation of the Cape Cod samples through a more rigorous quantitative evaluation and this is where making the connection to the modeling which I think would be a great next step. If we have these different iron phases, determine the surface area available for sorption from the tomographic images and then take that data and fit it into a more explicit surface complexation models or Kd models and compare the results to see how much it really matters for these samples. That's it.

MEMBER WEINER: Questions? Jim.

MEMBER CLARKE: This is kind of a general question maybe going back to the beginning. As I understand it, to me it looks like you're developing a framework. You're using particular species in your predictions and in your experiments, uranium for example and now cesium. How transferrable is this to other radionuclides of interest? If you know the chemistry, can you do that?

MS. ALTMAN: I'm going to defer that one for Randy.

MR. CYGAN: Welcome to the CMT work, the first part of the study really was emphasizing the mineralogy and I think that's clear cut how just identifying the fine coatings, the small thin-layered coatings, that occur on these substrates, quartz, feldspar, whatever. That's critical no matter what the radionuclide is obviously. Then with the cesium --

MEMBER CLARKE: My question was a little more general including the surface complexation modeling, the molecular modeling, just everything you've presented to us today. I just wonder how transferrable it is to be on the radionuclides that you focused on.

MR. CYGAN: Oh.

MS. ALTMAN: Each solute is going to have its unique characteristic.

MR. CYGAN: Essentially, you're not going to be able to just generalize their behavior. Obviously each system is going to have its own particular reactivity and association.

MEMBER CLARKE: That's what I said. If you know the chemistry.

MR. CYGAN: I guess you can make comparisons for analogous type behavior. If you go through the periodic chart, you can start to say like manganese and rhenium for example, that comparison. But I think going from the very fundamental molecular models all the way up it would be tough. I think what we could do is pick our targets carefully, try to make sure they cover enough of the periodic chart in terms of general behavior and then look at those trends.

I think there's a very specific problem. We'd probably want to do from the beginning. If you want to look at neptunium for example or plutonium, you could make generalities. But I think some of the behavior is very specific to that element especially if you're looking at the uniqueness of inner sphere versus outer sphere how many ligands are involved, looking at the hydration energies of solvation in the bulk versus pulling off those water molecules and trying to have it sorb on the surface is an inner sphere complex.

Those details certainly will require a lot of work. But I think you can make a map of let's say a dozen type of proxies and work on those to get that type of detail and then look at the trends.

MEMBER CLARKE: I asked the question for two reasons. Yesterday, we heard presentations on the new proposed EPA standard which proposes a compliance time of a million years. That suggests to me that attenuation in the subsurface is going to become much more important. Maybe it didn't need to be as important when the compliance period was 10,000 years.

Perhaps it needs to be looked at more closely now.

The other thing is that the radionuclides that drove the risk over a compliance period of 10,000 years may very well not be the same radionuclides that drive the risk over a compliance period of a million years. That was what really prompted my question. You've done some great work, it looks to me, on some particular radionuclides and there may be others that are going to be very important.

I guess the other general observation is you talk about going beyond Kds but you also talked about a way of getting much better Kds putting in water chemistry, surface complexation, modeling. I think that's going to become very important in PAs as well.

MR. CYGAN: Thanks.

MEMBER WEINER: Bill.

MEMBER HINZE: To follow up on your comments, it seems to me that this thermodynamic modeling is extremely interesting and very useful for characterizing the sorption on a variety of minerals under various physical chemical conditions. But being a geotype, I worry about how this really relates to the real world and how one takes into account the geological environment, not the physical and chemical environment but the geological environment and take into account the texture and structure associated with the compaction of clays, the occurrence of sand stringers in clays and so forth and how one can really apply this to a specific geological situation without having an extreme amount of characterization, geological characterization and material characterization.

That's an observation that I have that I'm wondering just how one is going to apply this. I can see this in the theoretical world, but I want to see this to the real PA world.

MS. ALTMAN: I think you bring up a really good point. The two issues involved, one is a scaling issue and the other is the heterogeneities in the system and you can't just dig out the ground and see what's in there. Traditionally, one way to approach it at the larger scale is you do, and I'm a hydro geologist, so I'm focusing on the hydrologic connectivities of porosity and the other materials that are important, the physical parameters important for the transport models, but you generate statistical fields. You take what you know from the well data of the stratigraphy. If you think there's stringers you can put things like that in a geostatistical model with a certain probability of them and you have to do numerous simulations and that's where you get your uncertainties and ranges of results.

MEMBER HINZE: Yes. You're absolutely right. The characterization on a variety of scales is extremely important to make this into a truly effective procedure.

MS. ALTMAN: Right. So the molecular scaling modeling, we have to take those results, build it up to a bench scale and see how well we can match that and then you go on to the next scale.

MEMBER WEINER: I'm going to take the liberty of asking a question because it follows right on to Dr. Hinze's. What steps do you think you still have to take or beyond these next steps, what do you plan to do to make this applicable to some of the problems that we have with the migration of radionuclides through actual natural systems?

MR. CYGAN: Can I defer that `till the next presentation?

MEMBER WEINER: Certainly.

MR. CYGAN: Because I have a summary slide in terms of future directions in mine.

MEMBER WEINER: Thank you.

MS. ALTMAN: But you brought this up

before. We have test sites with data and it would be great to be able to apply them.

MEMBER WEINER: Allen.

VICE CHAIRMAN CROFF: No.

CHAIRMAN RYAN: Again, I want to share in Professor Hinze and Dr. Clarke's comments that I think the work is fascinating, probably very helpful to getting something better than a shot in the dark Kd which I agree they can be all over the map. It's a well known parameter typically plus or minus two orders of magnitude.

But I urge you to think carefully about the systematic risks in your systems and in your measurements and in your calculations. There's a whole slew of them. It's not just an instrument, but it's a simple prep question. It's an instrument question. It's this question of backscatter and build-up in an x-ray beam. All those things are errors that you have to somehow systematically treat and then that's different yet again from a calculation uncertainty in a model.

The power of interpreting your data is only as good as a rigorous analysis of those uncertainties and I just urge you to think carefully about thinking about how you're going to go about doing that and I recognize as true experts in the subject your skills of interpreting are obviously at probably the highest level of anybody to do it. But you have to, I think, also add to that the rigor of a true statistical analysis that looks at every component of system error.

In my own area of interest, I often see folks that make a measurement with a gamma spectroscopy unit and they give me the error for the gamma measurement. That's typically the smallest error in the system and typically trivial in the system. Everything else is very important and typically ignored.

So I urge you to think about that and maybe add that kind of thinking to your analysis to make sure that you're not interpreting something that might not allow you to make that interpretation or you're distinguishing between curves that really aren't different. Just something to think about. But again, I want to emphasis. I think it's cutting edge work and very valuable to push in these directions to see if you can improve our use of these principles to improve Kds. Thanks.

MEMBER WEINER: Latif.

MR. HAMDAN: I also want to follow up Dr.

Hinze's point. The other risk that concerns me is the data that you have. Susan, you said you have it and you work with it. But the question before you do that is whether or not the data is enough to characterize the environment or the side that you want to characterize and that's a very important question.

MS. ALTMAN: Yes, I agree with that. You're talking about measurement there and you're talking about variability and they both have to be characterized.

MR. HAMDAN: So the point, sometimes data that you have is not enough and so maybe it's a waste of time to analyze it and deduce from it if you don't ask the question at the beginning is this data enough to characterize the situation I want to study.

MS. ALTMAN: And that's in part why the CMT data came in. They did the microanalytical techniques but they're time-consuming. There's a lot of sample prep. You can't do that for a large number of samples. So we're looking for -- And then you can go to batch structured experiments and get Kds. We want something a little better than that. So we're trying to find that something and it's doable to find the variability in it at the same time to get the details we need.

MEMBER HINZE: I'd like to point out that that variability is not just spacial but it's temporal as well particularly in the Vado zone and that throws an additional complication to it.

MS. ALTMAN: I agree.

MEMBER WEINER: Other questions? Hearing none, Randy. I suppose you're up.

MR. CYGAN: Okay. I'm going to finish up the Sandia part of the presentation for this morning and then Bill is going to end with some of the NEA project results. The last part, our task five is an emphasis on the memo of understanding that's among nine different federal agencies. This was started some years ago and we joined as representatives of the NRC.

We joined the MOU effort and we joined right at the time where they were preparing a reactive transport workshop. We had several people in our group who were quite interested in this and we decided to jump in whole-hog and we offered to host it. So we got quite in above our head in terms of dealing with a large group of people in trying to get a workshop together in a short amount of time. But the effort was all quite worth it.

This activity was defined in the May 2003 proposal. This is a Phase 2 proposal and I'll give you a webpage later on in the presentation which gives you the history of the MOU and of this particular working group. There are several working groups. One is for example that we've been involved in to a less extent is the one on uncertainty and uncertainty analysis. The other one is on reactive transport modeling. So working group no. 3 is the reactive transport one.

Our charge was to organize and convene this workshop and it was entitled "Conceptual Model Development for Subsurface Reactive Transport Modeling of Inorganic Contaminants, Radionuclides and the Nutrients." So it brought in a lot of other experts beyond the geochemistry people, the hydrologists. So we have a good audience for that reason.

It was held in April of last year in Albuquerque downtown and fortunately we had some financial support through the registration fees and some of the travel was brought up by these agencies. We had about 70 people who contributed who attended. These included people from the federal agencies themselves, academics and international as well.

Seventeen were invited speakers and we broke it down into four summary groups that had a little niche of each of the particulars of reactive transport. I'm going to briefly discuss what came out of the sorption workshop, sorption breakout session.

The workshop objectives were to confirm the needs and goals for field scale reactive transport modeling. I'm emphasizing the field scale here. Even though we're talking about in some of the presentations at that conference atomistic processes, the goal was to always scale up. So we're going back to the spatial and time scales in terms of the multiscaling.

We wanted to also demonstrate what the state of the art was in the discipline and how the modeling of the processes will control the field scale migration. This work was all in inorganic solutes. I'll be talking briefly about some follow-up work on organic materials.

What we were most concerned with in terms of the state of the art was to look at where the advances are needed in our scientific understanding, trying to see what the new approaches are for how we could develop better, improved conceptual models, assessing field relevant reaction parameters and also what are some capable, achievable targets for these new models.

This is just some eye candy if you will. It sort of represents the detail of what goes on in the subsurface and why this is a nontrivial, non-Kd if you will type of problem. This is a fairly nice schematic of the multiple scales that are involved in looking at a landfill on the margins of a river basin and how the leaf-shaped (PH) material can get into the subsurface and in this case, we show the complications associated with going through oxic zone and then into a reducing zone and then perhaps back into an oxic zone as it gets into the flow drainage.

We could also demonstrate the multilevel scale at least going back to what we talked earlier about, the atomistic approach, in this case looking at arsenic or iron and their valance changes as they are interacting with substrates or for example even colloid material and not just the sediment. That's a broad macro-scale, micro-scale, atomic scale and we heard this a lot throughout the workshop about Kds and Kd was often a so-called standard that was used for comparison of the surface complexation modeling.

Specifically to the breakout session on sorption and iron exchange, there were several recommendations. The first was to publish some guidance documents, something that the whole industry can refer to to establish pretty much what is the state of the art, what are the different choices that are available to the geochemical users or for that matter the licensee at some decommissioning facility as to make some judgment on how to go with sorption modeling.

The results on the matter of developing a new database for sorption model parameters. This goes well beyond the Kd but gets you into surface complexation models, site densities, equilibrium constants for all the reactions, acid/base reactions, complexation reactions and that sort of thing for not just ferrihydrite but for more common substrates. I mentioned earlier about Zomback Morrell (PH) references primarily for the ferrihydrite material. Then it was a material of also how do you extend a lot of the complexation modeling to more sophisticated systems and we talked about this already this morning is looking at vadose zones or infractured rock material. How easy is it to take more of the homogenous, uniform type application that we're used to for surface complexation modeling and try to push it into some rather unique type of environment but something that's much more applicable to some of the regulatory issues for the NRC.

The one unresolved question here was how do you make that third choice, Latif? We could talk about using something that's somewhere in between a Kd and a sophisticated SCM and that would be the generalized composite. How would any of these choices be most cost effective?

And I'd like to have the Commission recognize that Jim Davis in the Survey will be presenting next month hopefully and you'll get a better fee for how the generalized composite could be used as sort of a bridge which provides the rigor of the thermodynamic approach but yet reduces the number of parameters needed to model something rather complex.

And then the breakout session group also identified that there is a need for a field site to test all these, a field site that has somewhere a balance between complexity and tractability, a range of observable length scales with physical and chemical heterogeneity, things we've already talked about, also the effect of hydrologic and chemical transients, how a pulse might affect your modeling and trying to see the outcome of that.

And then also there was a concern about pretty much expanding this into all biogeochemical processes and that brings in an issue about the effect of bugs, microbes, and how they affect sorption processes. I know there are several groups around the United State, at least at the universities, who are really looking into the issue of microbial activity and how metals will be sorping certain exudates, polymers that are exuded from the bugs.

But anyway this field site issue and the complications associated with a field site, this was a common theme for each one of the four breakout sessions and not just our sorption and exchange.

MEMBER HINZE: Do you have any general reference on that biogeochemical work that I might be able to look at?

MR. CYGAN: The workshop actually had a breakout session that dealt with that and I have two sources for that. One is this document here which is proceedings from the workshop and then I'll be talking here about the webpages.

MEMBER HINZE: Great.

MR. CYGAN: One of our charges as host and for our Task 5 with the NRC was to develop public webpages for reactive transport modeling and this is the main page for the multiple agencies, the Steering Committee for Multimedia Environmental Models and this has a summary of each of the agencies that are involved.

Also it provides summaries of each of the different working groups. I believe there are four or perhaps five. I don't know if Tom's here or not. What's the count? Five I think. Four. Then part of our effort was coordinating the content webpages, providing public documents and then there was a publication of a Phase 2 proposal for our particular working group.

We essentially took our conference proceedings and got them into the webpage. This is all fairly minor stuff. Actually here you can see some of the different agencies at the time of the meeting who were involved. Actually, I should point out one thing that's been nice about this workshop is that we started to talk with the people in the USDA, the Agricultural Research Service, ARS, and the soil scientists there. So that has helped out tremendously with the collaborations and also it brought that community into a better working environment with the others in the field.

Essentially we have publications on the web of the abstracts, presentations and summaries of the meeting. This is the NUREG report that has all extended abstracts and short papers from the workshop and the summaries of all the breakouts sessions. That's to be published soon by the NRC.

There is also a nice workshop summary article that was published in the Transactions of the American Geophysical Union last fall which had a nice summary. In fact, the arsenic/iron example that cartoon was published in EOS, the Transactions.

The thing that we're working on right now, I'm working with Sabina Goldberg of the USDA and we're editing a special volume of the *Vadose Zone Journal*. I forgot the main editor's name and he's identified a special issue for next year to highlight reactive transport modeling, something that he sees as being critical and the people who are doing hydrologic modeling and trying to incorporate chemistry especially in Vadose zones obviously but it's fairly general across all groundwater systems and he recognizes that our reactive transport modeling, specifically surface complexation modeling, needs to have much more visibility in the community.

So we're going to be taking advantage of this and we essentially have eight authors who are from the workshop who will presenting in that issue. The lastly since the workshop, the emphasis of the working group has been on developing an organic subgroup.

Let me end with this last slide in terms of Sandia's interest and where we see things going not necessarily just by our group but other groups doing surface complexation modeling and that is to start looking at what level of complexity is needed to really apply to a particular problem be it a heavy metal contaminant or radionuclide contaminant. Now where do we have to draw the line in terms of how sophisticated of a model we need to really model it accurately?

Admittedly, a lot of our research has been emphasizing fairly detailed, fairly sophisticated methods either theoretical, computational or spectroscopic, experimental. We're not hiding that fact but this stuff is not cheap. It's somewhat costly but it's also using state of the art facilities. But yet we feel that it provides a good foundation or good bottom line for making judgment, especially legal judgment in some cases with NRC issues, on how best to do performance assessment.

So we don't hide away from that fact at all. However we recognize that in an application we have to draw a line somewhere. Some ways we might be able to do that is to perhaps look at a system where we know let's say critical substrates for sorption for radionuclides, let's say quartz, ferrihydrite and clay. Perhaps we could perform adsorption experiments and then fit the data using all the different sophisticated SCM models. Then we could look at the adsorption experiments, maybe just one or two or three at time, try to look at all the combinations and then compare that to assemblages.

So we do the minerals independently, apply the surface complexation modeling, bring in mixtures of the minerals, do the experiments and the complexation modeling and see how they compare to really prove that SCM can be a predictive tool. We have not done that yet. In fact, nobody has done it at this scale. So it's taking very fundamental monomineralic comparing that to mixtures and minerals and then comparing the complexation models.

CHAIRMAN RYAN: Just a quick question there. I think that's a good example of the kind of thing I'm trying to reach for. So basically you're saying you're trying to prove if it can be used for a prediction. What's the hypothesis driven experiment you're going to design up front to do that, statistically driven hypothesis?

MR. CYGAN: That gets to the point. If you're going to have -- We could demonstrate it perhaps for one or two or three as I mentioned here isolated cases. But statistically driven is a different issue.

CHAIRMAN RYAN: That's the key issue.

MR. CYGAN: That's the key issue but it determines how much effort you want to put into it.

CHAIRMAN RYAN: Without that though, I think you're kind of driven phenomenalogically and not in terms of your ability to reach your end goal which is to use it in PA.

MR. CYGAN: Right.

CHAIRMAN RYAN: So I'm struggling why that linkage isn't part of your thinking.

MR. CYGAN: The linkage is there but it becomes an issue as we start to prove the proof of principle let's say. If we can demonstrate that here is a single mineral and we could do the modeling perfectly on it. Then we take the same mineral, expose it in an iron solution and let's say we force out ferrihydrite on that mineral. Now we start to have a mixture of a substrate. Maybe it's quartz we looked at with minimal amount of sorption. Now we add an iron oxide component as a surface coating in a laboratory environment and if we could still predict the surface complexations for that next level of complication, then we have a building block to proceed to maybe two or three minerals in the assemblage.

CHAIRMAN RYAN: It's a big maybe.

MR. CYGAN: It's a maybe but it hasn't been tested yet. That's the hypothesis. Will it perform at the same level taking monomineralic data, combing them to a multiple soil mixture if you will.

CHAIRMAN RYAN: That's not really a hypothesis.

MR. CYGAN: No, not in its true sense of a hypothesis.

CHAIRMAN RYAN: That's again I strive to get across. That's what's going to tell you whether the research ultimately gets to the goal of really enhancing performance assessment.

MR. CYGAN: But at this level, my point that I'm stressing here is to do it right statistically driven will involve a lot more work than what we're proposing right now.

CHAIRMAN RYAN: Sure, and again an old mentor of mine said, "All the easy stuff's been done already." I hear you. It's a challenging problem but it's one that I think you have to face if you want to have the utility that you're reaching for.

MR. CYGAN: The next level of complexity on that sorption model would be to look at surface protenation (PH), something I only alluded to earlier, and that is if you're going to be talking about surface complexes and you want to have the detail needed to have these models be as general as possible, there's an issue of what is the protenation state and you could perhaps use these music or CD music models that are out there that would add that level of complication. But again, this is all at the very fundamental level and it's a big step to go from that into the application for PA.

There's certainly some clean-up work related to Geoquimico. I already alluded to those in the presentation earlier related to that software and I think that Susan just emphasized the issue about CMT. I think I'm going to leave it at this point. Obviously, there's some philosophical concerns about what's driving the research and setting up hypotheses. I accept that as a concern.

But I think the bottom line of our presentation this morning has really been emphasized that there are a lot fundamental physics and chemistry that go into these models that typically has been ignored. If they are included and to generalize in that way, we have a much more solid scientific basis to predicting surface complexation and attenuation perhaps to the point of intrusing to performance assessment codes. Do you want to open it up?

MEMBER WEINER: Are there any questions at this point? Latif.

MR. HAMDAN: Randy, have you thought or considered taking a study that used Kds for which you have enough data and try to redo the study with that surface complexation model and then not just one find, not just one study, maybe two or three studies that use Kds and see what kinds not necessarily to see which one is better but if nothing else to generate questions for you what it is that you want to pursue in the future. It seems to me if you look at three or four studies that use Kds and you applied your operatives the way you like to approach it, you would have some more meaningful questions as to where to go from here.

MR. CYGAN: A great suggestion as how you should go out comparing Kds and SCM. I would refer to Jim Davis and what the USGS has done. They're pretty much the field based part of our collaboration with NRC support. Jim Davis has been doing that. I think when you hear the results of the Naturita study, you'll be much more appreciative of the SCM versus Kd duality.

It's very easy to generate a Kd from SCM data. That's the baseline part of it. You can extract that out. You could see the variation in spacial and in temporal scales and they've done that in a really nice study with Naturita. So the data are there for the Naturita and that's what you'll hear next month.

With the same concern, they've also demonstrated that at the Cape Cod field test site and comparing tracer tests for example where they introduced tracer into the hole and into the well. So they're able to do SCM modeling of some of the tracers, either sorping tracer or non-sorping tracer, and they've done the comparison of Kd and SCM.

So there are a couple issues that I'm aware of. We personally are not the ones doing field studies and so I can't really answer that outside of referring to Jim Davis and their group.

MR. HAMDAN: The point I'm trying to make is that one important purpose of modeling, when you do a model, one of the most important purposes that's often overlooked is choose the model to identify where you want to spend your resources and you mentioned that this work is not cheap. So if it's not cheap, then the models are perfect for you to go and identify where you want to spend your money, where you want to spend your effort and use the case studies on Kds not so much to compare the surface complexation with Kd approach, not there, but in order to map for yourself what kind of things that you need, where you should go with your efforts.

MR. CYGAN: I agree. There are certainly some weaknesses that we aren't even aware of yet when we start to get into the applications especially a complicated application. Once we start to do that, we start to see where there are some pitfalls. That's when we have to back up to this type of level and we recognize that as being an ancillary or supportive role to doing the performance assessment which is to recognize where are the technical gaps. We can fill in those gaps.

But I will back up a little bit. This is an anecdotal story. The models are only as good as the assumptions. We've always heard that one. But a model has more than just the option being right or wrong.

An electrochemical Nobel laureate once

said, "A model can be totally irrelevant." That's the thing that we have to be careful of. We can't have a model that we push for performance assessment that has no bearing on the problem. It may give you a nice answer. It may give you nice graphics. It might give you nice, pretty pictures but it's totally meaningless. I'm afraid that in some cases we have pushed it to the point where it's meaningless data.

MR. HAMDAN: Thank you very much.

MEMBER WEINER: Bruce.

MR. MARSH: Why the fixation on Kds? I know it's a very convenient thing to use and people can get these results from various ways but why not go for rate constants so that when you formulate a model with differential equations and these things then can be put in and they're much more predictive and much more expansive in terms of the full regimes and doing many other things with it? Plus if you set the model up to begin with that has the right differential equations then it tells you what you need to head towards. I know you know these things and I'm just wondering if that's in your future direction also.

MR. CYGAN: Actually you brought us right back to the very beginning of our session this morning because I was emphasizing in the very first presentation this whole issue of being rigorous in the thermodynamics and to set up the equations properly, to use mass action laws, looking at equilibrium constants that go well beyond the aqueous system, that go into the substrate and the sorption process. So that's definitely the whole background. I don't know if you were here at the very beginning.

MR. MARSH: I wasn't.

MR. CYGAN: But certainly we recognize that that is the advancement that we're pushing towards. The application of the SCM is to base it on that. We reference Kds here primarily as a reference. The Kd has just been the norm in typical hydrology PA codes and it's the simply way out to describe all the chemistry.

We know pH, ionic strength, composition, multiple substrates, the surface state of that substrate are all critical issues that can actually be addressed in very rigorous manner with the thermodynamic tools that are out there and the extensions of the thermodynamic tools. So I appreciate you rallying around that point because that is the main emphasis of our work. The Kd just happens to be a point of reference for comparison for PA codes.

MEMBER WEINER: Just to move things along, I think, Bill, you had a final statement. I'm sorry. Go ahead and ask your question. Dr. Hinze, go ahead. Okay. We defer.

MEMBER CLARKE: Just a quick question.

MEMBER WEINER: Well, you cut Bill off, but go ahead if it's quick.

MEMBER CLARKE: Just very quickly here. Are you planning any future workshops?

MEMBER WEINER: The question is invite us. Let us come.

MR. CYGAN: Unfortunately, we didn't do a good enough job advertising the last workshop. There are a couple of representatives here from the NRC who were there and I think some of the other people in the audience. We have nothing planned. I don't know what the state of the other MOUs are but those are annual or biannual events and I'm sure surface complexation modeling will be discussed, those MOUs, as part of the working group meetings.

MEMBER WEINER: I might say that Bill and Susan will be ready to answer any questions that you pass to them by email or call them up or if we have further questions. Bill, you had a final word.

MR. OTT: I have the NEA project.

MEMBER WEINER: Yes, the NEA project review.

MR. OTT: I'm going to go a little bit farther now and discuss the last thing that Jim Davis was going to discuss, the NEA sorption project. That's the OECD Nuclear Energy Agency. It's a project that involved on the order of 16 organizations from 13 different countries and it has had two phases.

The first phase was basically do we think we can do any better than Kds and the actual observation remark to Bruce is that the problem is that every PA model that I know of uses Kds. That's primarily why the focus is trying to evolve from Kds to something better. Kds is sort of the reference where we are and we don't want to be and the question is how do we get someplace better.

Anyway, the first phase decided to the surprise of some of the participants and some of the member countries who had placed a lot of effort in the Kds and really didn't want to go away from it that there had been considerable scientific development over the previous 10 to 15 years since they started doing it and perhaps they should be thinking about doing something better.

The second phase of the project was to

actually look at what's out there and do some comparisons. So they did was they took these participating countries and organizations, developed a benchmarking study and the benchmarking study involved six or seven technical cases that were developed by a technical direction team. Jim Davis's group at USGS was our modeling team but actually the NEA asked him to come on board and actually head up the technical direction team.

So this group selected test cases varying from fairly complex information on Naturita to just single mineral studies. The teams from these various countries modeled these test cases. We had 16 modeling teams modeling seven different test cases. You rapidly get a fairly large number of test case analyses that this particular modeling project undertook.

In the end, they published this documentation which I've given the reference to Dick. It's available through the NEA and unfortunately they're very tight with the copies they put out.

In this particular document, the NEA Sorption Project Phase II, Interpretation and Prediction of Radionuclide Sorption on the Substrates Relevant for Radioactive Waste Disposal Using

Thermodynamic Sorption Models. I haven't read it entirely myself. I glanced through it and read in detail certain portions of it. It's a very good summary of the state of the art of what can be done and it's very interesting in attending the final workshop and listening to the technical direction team on what they did and didn't do.

One of the things they discussed and didn't do was constrain the modeling teams because they wanted to get a feel for how people out there how adept they were at interpreting systems and applying these thermodynamic sorption models. In the final result, they found that they had a wide range of response just because they didn't constrain it because some of the teams actually came in trying to learn how to do the process and came in from a fairly naive perspective. All of this reflects on the results that they published in here.

Now let me go to the actual slides themselves that Jim provided. Some of these background things I won't go through, I won't emphasize a lot. The bottom bullet on this slide "Nearly always management organizations use Kd in their PA calculations."

Another aspect of this workshop that we

just held over in Paris was that not only were the participants in the sorption project present but they also invited PA modelers from a number of the agencies and they invited members of the IGSC which is the Integrated Group for Safety Case which is a higher level NEA committee which is looking at performance assessment among the member nations in the whole. So they had the PA modelers and the IGSC people there.

And later in the week there was an IGSC meeting in which they discussed the results of the sorption project. All of this stuff was coming together and coming to a head. The question involved was whether the NEA thought that they should continue to do work in the area of sorption.

There's a general desire to have a scientifically robust and defensible basis for these geochemical calculations. They know that the old constant Kd view is wrong, that Kd isn't constant, that that fraction varies with chemical conditions, with solution compositions, the nature of the amount of solid materials, the wetted surfaces. They can vary from point to point and Bill's observation about what about all this fine structure in the geological environment is well taken. I think we recognize that.

As a side comment, I wanted to refer back to the presentations you had last summer about model extraction from the Agricultural Research Service in which one of the basic questions we're trying to address is what is the appropriate level of complexity to employ in any given modeling situation. Maybe it's isolated and it's just a short pathway within a larger medium. So that question of what level of complexity is one that we are addressing in another part of the program.

The people that put together the sorption project felt that confidence in Kd values used in Pa would be improved. If we can show that there's a basic understanding behind these Kds, behind the values that are used, behind the way that those values are derived. The observation that they're not transferrable. If you just take the concept of Kd and measure that at one location, it's not transferrable to another location because the conditions are different.

What Randy has done in terms of trying to look at the basic mineral phase and the radionuclide species, it should be transferrable. The question is how low can we go and how can we build that into a larger system.

I'd already mentioned this. Eighteen

funding organizations, 13 member countries. Trying to reduce uncertainty in Kd. Reduce increased confidence in PA. This is the bottom line for all these NEA countries. They want to increase in their performance assessments. That's the only reason they're funding this work and trying to improve this is to increase the confidence in those PAs.

Hence we went into the intercomparison exercise. This talks about the benchmarking exercise which I've already told you about.

Now we're going to go basically into the results. This is a large document but you'll see some commonality between the results here and the results that came out of the workshop that we had at Sandia. And you have to realize this is focused only on sorption. The Sandia workshop was focused on reactive transport in general and only one of the breakout session was focused on sorption. As Randy mentioned, results of the other breakout sessions are available on the website and will be available in the draft NUREG when it gets published.

The key results from the Phase 2 report. They feel that the robustness of the basic concepts underlying thermodynamic sorption models represent phasion (PH) of radionuclide Kds. They feel they have a good demonstration in here that using a more defensive and more scientific approach, using thermodynamic sorption models they can reproduce what's happening far better than you can with a constant Kd and they showed this time and again in test case after test case.

Another thing that came out of the workshop was they thought they had in increased awareness of critical issues and that improved communication and scientific defenseability for these models and between the modelers was very important.

As the Sandia workshop said, they think that the establishment of model guidelines with respect to thermodynamic sorption models for use in the safety cases not only is needed. They think it's now feasible. They feel that the conclusions that they've reached and the general trends that they saw in the application of thermodynamic sorption models to all these test cases have real and significant information that we could coalesce into a reasonable guidance document on the use of these techniques at the current state of the art. And that's the last bullet.

This was generally with regard to the range of test cases involved. Advanced modeling strategies are feasible with less complex materials dominated by one or few defined minerals. The generalized modeling strategies are suitable for quantifying sorption characteristics of complex materials. I'm not a geochemist. I'm not going to try and explain those any better than that right now. You can hit Jim with that when he comes in in December.

Potential issues and actions for a possible future program on TSMs for supporting -- These are identified needs that came out of this and here we say it again. Developing guidelines for TSM model development. That's model development for a given application.

How do we address a specific application? Ensuring model, physical and chemical reasonableness. Proper quantification and assessment of errors and uncertainties. Mike's issue. Upscaling criteria and credibility. Moving from lab to reality. Bill's issue of how we go to larger systems. This is something that came out of the sorption project.

Here we go with education of PA modelers, performance assessment modelers it should be, about TSM application to relevant systems. I think you're seeing that we're coming to a lot of the same conclusions and answering the questions that you raised here. We see the same weaknesses you do and the sorption project I think they're identifying to NEA that we ought to support further work to do this.

MEMBER HINZE: I'm curious though. Randy mentioned the organics. How much are you involved in organics? Have you evaluated whether they're important to study? Where do you stand in that?

MR. OTT: The work on the NEA sorption project is looking only at radionuclide sorption. It's not looking at any organics at all. To the extent that the organics might be the source of carbon in the system and the carbonate reactions, of course it's important. There was much more in terms of general organic stuff at the workshop in Sandia.

MEMBER HINZE: But this is not something that you're focusing on.

MR. OTT: It's not a focus of this particular project.

Possible actions here are actions that are going to be proposed to the NEA. And it's a document describing a strategy for development of TSM models for a wide range of materials and chemical elements of interest to PA written in a manner which facilitates communication of use of TSM and supportive Kd in safety cases.

This is again this issue of documentation. We've begun to see some indication that our licensees would like to use more advanced processes. We're also seeing some indication that we don't know how to do it. It's critical if we want to move forward and have a more scientifically based use of these processes to evaluate sites that we need to development somewhere some kind of guidance on that.

We're working on trying to put together something in-house, primarily an internal document for internal guidance. We haven't gotten it thoroughly scoped out yet and it's one of the things I want to talk to Randy and some of the staff about this afternoon.

But we would be hoping that if we do something like this we might actually submit it to the Working Group 3 of the MOU for other federal agency interaction. If the NEA does come up with another project to Phase 3, then we might provide it to them as a starting point, a point of departure for this more extensive document.

Unfortunately, it takes awhile to get things started with the NEA. They'll come down and ask somebody to write a proposal and the proposal will go back. The proposal get reviewed. It could be anywhere from six months to a year before anything else gets started. And we feel a need to at least derive some benefit fairly soon from this work because the indications are that there is enough there to get some significant benefit right away.

Then the last bullet on here is a training program about TSM application to relevant systems. So the NEA is saying if we develop the document then we ought to provide to NEA members training in the use of the techniques.

MEMBER WEINER: Thank you very much. I'll go around one more time. Bill, further questions? Allen?

VICE CHAIRMAN CROFF: I think I will. I think you maybe have implied this but I want to be explicit on it. What I'm hearing from you is these models in your opinion are ready for prime time. In other words, they're practical for use by people out in the field outside of a research setting.

MR. OTT: We've reached the point where in cases they will be. This is a very complex subject and sites differ very greatly in the amount of information available on individual radionuclides, on individual mineral species and how those species and radionuclides and other chemical complexes interact is highly variable. In other words, you may have sufficient information at one site and not at another.

This is where, I hate to keep referring back to Jim Davis's project and I wish he had been here today. This is why the approach that has been used in Naturita is fairly crucial. In being a semi-empirical approach, it probably makes more use of onsite data than you might use, say, 20 years from now if you have an established database.

The other thing that was mentioned in here by both Randy and by the NEA was the need for a database. The databases that are out there now are incomplete like you've mentioned this Zomback Morrell is only for the ferrihydrite. That's not the only substrate that we need to have the data for in order to apply these models on a general basis.

The generalized composite approach that Jim is using essentially tries to study a site and come up with a set of basic reactions that characterize that site and he'll arrive at those reactions from characterizing the mineralogy of the site and the basic water chemistry. What he'll do is he'll look for those reactions that he feels will dominate the system.

Then he'll go back and he'll do a site specific application of this work that essentially fits a lot of the constants to that site and the reason why it's a semi-empirical approach. It's not the Kd which does the same thing because it includes a lot of the actual reaction chemistry that's involved. But it's also not the full-blown surface complexation model that realizes on the complete knowledge of the mineral substrates and the contaminants. It's the in between approach that Latif was talking about.

VICE CHAIRMAN CROFF: And you can write down criteria defining which kinds of sites it should be used for and which ones it shouldn't be used for.

MR. OTT: I think that based on the information in the NEA report and the other work that's been done by USGS and the Sandia we could probably provide guidelines. I don't know if we could come as far as criteria, but guidelines as to how to approach a given site in any kind of given environment.

VICE CHAIRMAN CROFF: Thank you.

MR. OTT: I think we're at a point where we can do that.

MEMBER WEINER: Bill, a couple of

thoughts. One is I think the committee has applauded your efforts in the past and I recognize now that you're leveraging limited resources for this kind of research by participating with other federal agencies and internationally and I think that's something we recognize as having great value and you're really stretching your dollar and getting the most out of it that you can. I think that's terrific.

The second is I'm really taken by this exercise aspect. I'm reminded of years ago at Oak Ridge. Mixed field dosimetry was magic for a long time, neutron and gamma ray dosimetry, and I guess it was 25 years or so that an international intercomparison of dosimeters was actually conducted every year at the Dose-R Reactor which was a burst mixed field reactor.

It was fascinating to see those results over time. It was kind of like you described your results. There were new folks. It was kind of all over the map but as that group routinely met every year, they found the central tendency after awhile and there was an awful lot of learning that went on by seeing other folks' results.

That's a great activity I think because it really gets you at the point where you can say I'm on the center or I'm out here in left field with my model whatever my model might be. So there are some really good examples in the past where that kind of exercise works. Is there any other activity on this NEA sponsored activity to do this kind of intercomparison?

MR. OTT: This is the only one I know of at the moment.

CHAIRMAN RYAN: Should there be an effort among the federal agencies in the U.S. to do it a little bit more provincially for the U.S.? You don't have to answer it today but it's something to think about. I guess I find that prospective pretty exciting because it really is a way to sort out all of these issues whether it's my uncertainty questions or some of the other ones to really get down to the brass tacks and begin to do it in a forum that's not a licensee trying to meet a requirement. It's more of an open forum to look at the issues on their own merit.

MR. OTT: The interesting part of the NEA exercise is that you have so many countries that have waste management programs right now.

CHAIRMAN RYAN: Sure.

MR. OTT: And actually if you look domestically, we don't have as many single-goal programs out there that might be interested in an intensive benchmark study like this. Maybe we do. There are a couple of agencies that are interested in a couple of states but I don't know that we could generate the same level of intensity that we had in this particular project.

CHAIRMAN RYAN: But by the same token as you pointed out, the NEA wheel turns a little slower than it might here.

MR. OTT: We have found ourselves to be something of a forcing function. We force the MOU and we actually force the NEA a little bit here.

CHAIRMAN RYAN: If you can see strategies along those lines that you think we could be helpful on commenting on, we'd be happy to hear about it.

MR. OTT: An interesting aspect of this that you remind me of is that because we had this range of application expertise they also deduced a lot of things about faults and ways that you can go wrong. So there are all sorts of insights in this document that I think could be transferred into guidelines that would be very helpful.

CHAIRMAN RYAN: And again, I think those intercomparison efforts you're multiplying your own work by however many participants you have and it's usually a pretty high return.

MR. OTT: I have to also give some other credit. You haven't asked the question about how we're transferring this work to NMSS or whether the high level waste program is involved. One of the modeling teams in the sorption project was from the Center. We specifically invited NMSS to participate in the project and they funded a modeling from the Center. So they participated in the NEA sorption project and they sent two people over to the final workshop. Goody (PH) was there and Dave Turner.

MEMBER WEINER: Goodness. You answered the question before I asked it. Jim, do you have further questions?

MEMBER CLARKE: You mentioned that it's considered to be feasible to develop model guidelines for the TSM models. Is that work going forward? I couldn't tell if that was.

MR. OTT: This was a conclusion that was expressed at the workshop in Paris which occurred about a month ago. As a matter of fact, it was Scott Altman that was the one that actually came forward and said that he felt that based on the summary report of Phase 1 and Phase 2 it is now feasible to provide some kind of general guidelines that would be helpful in applying these models.

MEMBER CLARKE: Would those guidelines also address the data you need to most effectively use the model site characterization aspects of the models?

MR. OTT: Yes. It would have to address all those aspects.

MEMBER WEINER: I just have a comment and that is we have successfully used basic chemical principles in PA and I encourage you not to give up that focus. We did it for the waste isolation file client and it's also been done in some of the PAs that have been done for Yucca Mountain as well as other sites. Looking at how one applies these very basic principles to a PA, to the calculation of some sorption model, I think is an effort that is certainly worth completing and coming to some conclusions for. I don't want to mess with that at all. Does anyone else? Latif.

MR. HAMDAN: Really quick. If the guidance and the database were to be developed, who would developed them?

MR. OTT: The NEA right now is seriously considering the database issue, the database that Randy referred to before on the aqueous speciation (PH) is an NEA database and if the IGSC and the other countries look at the evolution of the process and feel that this is the way of the future, it seems to be a forward looking enough organization that they would consider doing that. That is not a trivial task as I'm sure you know.

MEMBER WEINER: Other questions, anyone? Hearing none, I'll turn the chair over to the Chairman.

CHAIRMAN RYAN: Thanks, Ruth, and again, thanks to all the presenters and the discussion this morning. It's been real helpful and interesting and as I said, all the easy problems have been solved already. So on we go to the tougher ones. But I think the fact you're leveraging the work with many others on an international scale is really a fabulous way to go about it. It will hopefully bring us answers quicker rather than slower. So great job.

A couple of housekeeping items. Based on the shift in schedule, we're going to take up some letter writing directly after lunch. I'm going to suggest we come back at 1:15 p.m. instead of 1:30 p.m. and we'll start with the igneous activity if that suits Professor Hinze, followed by Allen's letter on the West Valley Performance Assessment.

We will then move on schedule to the Low-

Level Waste White Paper because we do have a participant by telephone. So we have to maintain that schedule. But we'll pick up whatever letter writing doesn't get done after that short one hour or shorter session on the White Paper.

MEMBER WEINER: You mean the SRP for Allen.

CHAIRMAN RYAN: Yes. I'm sorry. So we'll do those two letters that we have right after lunch starting at 1:15 p.m. We will not need the record until 3:00 p.m. when we have the session on the Low-Level Waste White Paper and we'll proceed on from there. So again, thank you all very much for your participation. We'll see you at 1:15 p.m. Off the record.

(Whereupon, at 12:05 p.m., the above-entitled matter recessed to reconvene at 3:04 p.m.)

A-F-T-E-R-N-O-O-N S-E-S-S-I-O-N

CHAIRMAN RYAN: On the record. Tell us who we're tying in please sir. Is it Alan Pasternak?

MR. PASTERNAK: Yes.

CHAIRMAN RYAN: Yes, Alan Pasternak from the CalRed Forum. Thank you.

(Discussion off record.)

CHAIRMAN RYAN: We're in open session and we have a transcription going, Alan. So welcome and Alan Pasternak from the Calred Forum is on the phone and I think we have your participation duly noted. Alan, I don't know if you have in front of you but we'll be happy to fax it to you something that's on the screen which is the outline of this Low-Level Waste Paper. But before we get to that, I just thought I'd make a few introductory comments and again we'll have comments from participants as we might go around. So if you need to say something, chime right in. Okay?

MR. PASTERNAK: Okay.

CHAIRMAN RYAN: All right. Several meeting ago, six months or so ago, we undertook to think about the history of low-level waste and its regulation and this is a first step and the step that we're going to talk about today is the report.

Are you on a speaker, Alan?

MR. PASTERNAK: I'm sorry.

CHAIRMAN RYAN: Are you on a speaker phone?

MR. PASTERNAK: No, I'm not.

CHAIRMAN RYAN: Okay. Because we're getting just a little bit of static from you, but we'll see how that goes.

We developed I hope what is an accurate history of low-level waste regulation in the United State. We decided on taking this tactic of being fairly rigorous in trying to document the entire history of how low-level waste has been regulated over time and it's parts and pieces so that we can better have insight into how the definitions that currently exist in low-level waste spring forward into other areas of waste regulation and even nuclear material regulation.

Where we are in the report development process is that we have a working draft that is probably 98 percent or so along the way to completion. I'm going to ask Mike Lee in a minute to talk a little bit more about it. But as we finalize that draft and just clean up all the little spots where we have to get a reference and do a final editing check, we'll then make the report available as we report it to the Commission. So that will be coming along.

In short, what we tried to do is cover several parts. The first two parts are the low-level waste program history and we started from the very earliest days of the Atomic Energy Commission, talked a little bit about ocean disposal, land disposal and early performance issues and then a bit of the Congressional history for 10 CFR 61, the Low-Level Waste Policy Act of 1980, the Amendments Act of 1985 and in efforts, we've covered the issues of efforts to cite new disposal sites in the United States and the current program status.

The second part was to review the NRC low-level waste regulatory framework from the development of Part 61 including the basic questions of who should be protected and what should the level of protection be, some of the scoping activities that occurred in 10 CFR 61 including NUREG 0456 which was titled a "Proposed Low-Level Waste Dose Assessment Model," NUREG/CR-1005 "Proposed Radioactive Waste Classification System" onto NUREG 0782 "The Low-Level Waste Draft Environmental Impact Statement." I think it's interesting to note the Draft EIS is the one where the intruder scenario is most explicitly described in terms of the doses that were assumed and the various assumptions that went into the actual scenario that I guess could be viewed as a bounding case at least and maybe even an extreme bounding case if you consider some of the details of how that intruder had to conduct its life to be exposed, including waste streams that were considered and of course exposure pathways that were considered. All that information we tried to summarize and in fact document from these foundational documents.

The definitions of safety we've tried to capture what EPA has said in regard to its promulgation of generally-applicable standards, NRC selection of a default low-level waste standard and the Waste Classification System that came from the EIS process into the final EIS and the regulations subsequently. Then there, of course, are other regulatory developments including guidance and strategic planning.

Part 3 which is empty at the moment is ACNW's observations and recommendations and I think after we all have a chance to study the final document, we'll be having an open session where we'll talk about what our views and thoughts are on observations and recommendations that may come from this hopefully detailed and thorough study. Several appendices will be included, a study of the structure of 10 CFR 61, the final Commission policy statement on the use of PRA methods in nuclear regulatory Activities, the regulatory evolution of the definition of low-level waste and then a summary of the past ACNW advice and recommendations in our previous letters in the area of low-level waste.

Again our goal is to try and produce a comprehensive package of information in one place so that any discussion of low-level waste from this point forward will be on the same footing for anybody that reads this document.

We have one table also attached for everybody's consideration today and that is the potential candidate areas where we could think about how could 10 CFR 61 be improved. This was taken from Attachment B of an NRC 1993 analysis on that topic. So this tells you what the NRC at least was thinking some 12 years ago or so and there's a list of those. I won't go through each one but such issues as active maintenance, performance objectives, technical requirements for land disposal facilities, sites suitability requirements, environmental monitoring, land ownership, institutional control period, waste classification and characterization, retrieveability option, groundwater protection requirements were all things that were considered at that time.

Again, I think the overarching view is that we tried to not necessarily interpret anything but rather not interpret things at this point and get a very accurate, complete factual history down about where low-level waste has been in the last 45 years or so. Mike, anything to add?

MR. LEE: No, Dr. Ryan. That was very comprehensive. What I did is like Dr. Ryan said, we tried to at least in the first round of writing just present in essence a literature review just stating the facts of what was done and why. We tried to reference it as extensively as we could to make our sources of information transparent. There's still a little bit of bird-dogging on some references and a little bit of writing here and there to do.

I'd like to clean up Section 7.1 a little bit. I'm not happy with how my first crack at the writing went on that and Appendix C, the regulatory evolution of the low-level waste definition, still has to be hammered out, but I don't think that's a substantial effort. Former alumnus Howard Larson has been tasked to go ahead and develop a draft of

Appendix D which is a summary of the past 19 letters the ACNW wrote.

CHAIRMAN RYAN: Just for those who don't know what a former alumnus might mean, you might explain how it's a former job and that we've retained him as a consultant.

MR. LEE: Sure. Howard's a former support staffer with the ACNW. He recently retired and has come back, has been rehired. So that's really about it, I guess. What I did do though is we put together a table which Dr. Ryan alluded to which is Table 14 and this was an earlier analysis that the staff did in 1993 that identified potential areas for consideration of revising the regulations.

The one recommendation I didn't include in here which is addressed in the text of course was a recommendation to go with a risk-based performance type of standard with just performance goals and no technical requirements per se. That's covered in the writing here.

CHAIRMAN RYAN: So with that introduction said, I think the steps that will occur from this point is we'll report this summary to the Commission and then of course, we'll finalize it as a public document concurrent with that submittal. I think we'll be in a phase then of welcoming any and all comments on this history to make sure that we haven't missed anything or misrepresented any particular detail or that we have everybody's views on what the history actually is and we get all those facts right. Then I think the Committee will begin its deliberation and again those will be in open sessions to consider views, inputs or other opportunities to get views on what should change, should it change and how should it change to perhaps improve the process or the definitions of the regulation of low-level waste.

One item I just might mention as a view that developed yesterday in our session is that we heard that the plan for 10 CFR 63 is that the worker dosimetry will use more modern ICRP dose factors and waiting factors in particular. That would be different than what's in 10 CFR 20 and I note that the dose basis for what's in 61 is also different. That relies on ICRP-2.

Instead of having two foundations from ICRP, one from 1959, that is the ICRP-2, we would end up with three. Depending on where the worker worked, you would end up with three different views of -- Not where the worker worked. Where the dose is calculated for a member of public for low-level waste and workers for Part 20 regulated facilities and then for Part 63 at least that prospective dose would be different.

So that's just one area where it's worth thinking about. Is there an issue there? Should something be changed? Is it okay the way it is? I think that's just a small indicator of the kind of things we'll be thinking about. Comments? Questions? Jim? Anything? Ruth?

MEMBER WEINER: Does the title of Table -- Are we on the record?

CHAIRMAN RYAN: Yes, we are.

MEMBER WEINER: Does the title of Table 14 Potential Candidate Areas to Amend in 10 CFR 61, does that imply that we may be considering recommending changes to the rule itself?

CHAIRMAN RYAN: No, that is what was considered in 1993. That does not reflect anything that we're considering. That was taking from a reference. So thanks for clarifying that.

MR. LEE: Right, and I've included that source document in the little blue folder I gave you there. So if you go to Appendix B of the `93 memo from the staff to the Commission you can see exactly what the staff wrote.

CHAIRMAN RYAN: And again, I want to

recognize and thank Mike Lee and Sharon Steele for both their efforts on pulling this document together. Sharon did some of the early ground work in pulling the huge chunks and parts and pieces together and Mike's done a lot of the writing to organize it and I appreciate both of your efforts. It's an effort well done. Any other questions, Ruth?

MEMBER WEINER: No, that was my question right now.

CHAIRMAN RYAN: Allen.

VICE CHAIRMAN CROFF: No.

CHAIRMAN RYAN: Bill?

MEMBER HINZE: A couple. What's our timeline on this?

CHAIRMAN RYAN: Correct me if I'm wrong but I believe we'll probably be turning it in December 31st, by December 31st. So I think we'll finalizing it probably at our meeting next month.

MEMBER HINZE: The second question is where do we stand here with a discussion of time of compliance in low-level waste.

MR. LEE: In Appendix D, Howard was going to go ahead and take a crack at organizing the 19 or so letters. You recall that previously we compiled a list of all ACNW letters and in all the areas --

MEMBER HINZE: I wrote it. Right.

MR. LEE: -- we tried to organize them by topics.

MEMBER HINZE: But it's more than that. It's more than the ACNW's views. It's the background in the whole are of time of compliance. Isn't there a role here?

CHAIRMAN RYAN: In the `61 regulation itself, there's a very limited bit on time of compliance. It's not a topic that's taken up even by that title or subject.

MEMBER HINZE: But it's there and it's an important element.

CHAIRMAN RYAN: It is there subsequent to the regulation. So the letter is as probably as good of a history of it is as there is. Now should we look for some more? Absolutely. We'll take that up.

MEMBER HINZE: And I guess my concern was that I don't believe that should be relegated to an appendix.

MR. LEE: Just for a little background, do you recall that in the mid `90s and maybe `96 the Commission issued its Commission paper on its six performance assessment related issues, one of which was how long the PA should be conducted for a low-level waste facility? That's included in the body of the text but the intent wasn't to give short-trip to the past Committee advice. We can work that in as a --

CHAIRMAN RYAN: Yes, I think just for convenience the letters will all be in the appendix. Then the discussion of it will be in a section in the body of the text.

MEMBER HINZE: Sure. And that's all that I would like to see.

CHAIRMAN RYAN: Fair enough.

MR. LEE: We've been moving fast.

CHAIRMAN RYAN: Again, we have a number, I think, folks in the audience who are interested participants in low-level waste activities in one way or another. If there are any other comments, we'd be happy to have those at this point and the brief summary of previous thoughts is available through Mike Lee and I think we have copies for folks. You're shaking your head no. It's not available or you have nothing to add.

So at this point, that's probably where we stand and I just wanted to give everybody an initial view of how this is shaping up and what the outline of the report looks like and we're going to go on from there.

MR. PASTERNAK: Dr. Ryan, this is Alan Pasternak. Is this an appropriate time to jump in?

CHAIRMAN RYAN: Yes, please sir.

MR. PASTERNAK: I just want to express a point of view of organizations that use radioactive materials. What is needed in the low-level waste area and urgently needed is access to more disposal facilities. From our point of view, there is no crisis or urgency with respect to the regulations themselves. They've been on the books now since about 1982 and they appear to be working well. 10 CFR 61 appears to be working well.

The problem as I'm sure you know is loss of access for disposal of B & C waste by organizations that use radioactive materials in 34 to 36 states and that will come about July 1, 2008 and also the prospective that as of the same date, there will only be one facility in the country to which these same organizations can dispose of their Class A waste. So you have monopoly control.

I was glad to hear your response to Dr. Weiner's question that you're not planning a revision to the regulations. We think such a revision would only delay solutions to the current impasse.

I would respectfully refer the committee to several statements on the record. One is the comments of the Nuclear Regulatory Commission itself on the June 2004 report of the Government Accountability Office to the Senate Energy and Natural Resources Committee in which the Commission calls for some changes in the national framework in the interest of providing assurance of disposal availability to organizations that use radioactive materials, assurance and stability in the framework.

Then there is also a position statement of the American Nuclear Society and more recently some very strong position statements by the Health Physics Society. I hope that these are reflected in the ACNW's report because these all point to the critical issues with respect to low-level radioactive waste disposal.

I don't know. Is the current draft available to the public?

CHAIRMAN RYAN: It is not yet because we're still in the final writing stages. But in the spirit of wanting to be open and forward in our thinking here in this forum at the ACNW, we wanted to go through the outline that we had to-date and I might just ask if you could scroll down past Section 7.

Mainly the focus was to get all the regulatory issues correct. Alan, you've raised a really interesting point and I think there are sources of information that are contemporary at least across recent times and us thinking about and studying position papers and the GAO report and Commission comments on that report is an excellent suggestion and we'll certainly add those.

If you have other suggestions on those kinds of related documents, we'd be pleased to make sure that we give those full consideration in our deliberations as well. So that's a great suggestion. Thanks. I think we're all aware of them but including them formally is a very good idea.

MR. PASTERNAK: Yes, and again in the area of low-level waste disposal we think the crucial issue that the ACNW hopefully will focus on is the need for access to more disposal facilities and disposal options for all of those organizations, governmental, private, commercial that use radioactive materials.

CHAIRMAN RYAN: I think at least my view is that we certainly can be mindful of your thoughts and interests in that area. But again, I don't think we have the power or authority to make specific steps toward those goals. But we certainly can understand your perspectives and ideas on them, your views toward those goals. Again, I appreciate your input and suggestions. Mike, you had a comment.

MR. LEE: Yes. The GAO report in question has been referenced in the report.

CHAIRMAN RYAN: Right.

MR. LEE: We can certainly go back and see what we had to say about it. If Mr. Pasternak has any recommendations on stakeholder views or organizations we could reference that had public views.

CHAIRMAN RYAN: I think there are two, the ANS and the HPS statements are public.

MR. LEE: Okay.

MR. PASTERNAK: Yes. There are others. There's a Council on Radiopharmaceuticals and Radionuclides. There is a more recent GAO report issued in September of this year, GAO 05967 on Sealed Sources and that also has some interesting comments on a possible role for the Department of Energy.

CHAIRMAN RYAN: Again, any other society or professional organization position papers that might become available, we'd sure be happy to be informed about those. It leads me to think as well, and I'm thinking out loud here for the moment, but we ought to understand if there's anything that the CRCPD or the Organization of Agreement States has commented on or has a position on in this area. I don't know that they do but I'm just trying to check that box as well.

MR. PASTERNAK: Okay.

CHAIRMAN RYAN: Anything else? Alan, you have the floor still.

MR. PASTERNAK: No, I think I've said what I wanted to say. Thank you very much.

CHAIRMAN RYAN: All right. Thank you and unless there are other comments. Yes, we have two. Would you please speak in the microphone and identify yourself and your organization?

MR. LIEBERMAN: Jim Lieberman. I'm here representing myself. Are you going to consider international developments, IAEA documents, that talk about different types of waste systems?

CHAIRMAN RYAN: Jim that's a good question. I guess in my own thinking we had sort of touched on it. But the framework of some of the international systems is a lot different because they have high-level, intermediate-level and low-level and the scheme doesn't line up. So we would be kind of in a constant translation scheme. So while I think some of the general documents, for example you mentioned the IAEA ones, are certainly instructive and I think have some good science and good things to think about, I think they tend to be general enough to where I don't know that they would add a whole of lot guidance to this much more specific evaluation.

If there's something that you could identify that's very specific that you think does have particular value to this agenda and our table of contents in the subsequent report, we'd be happy to have a comment in that regard that this IAEA report or NEA report or some other report had particular value. We'd be happy to think about that.

MR. LIEBERMAN: I recognize what you're saying, Dr. Ryan, but I was thinking one general point you might make is the fact that in the international community they're looking at the different levels of classification very low-level waste, intermediate and the fact that they have different categorizations with different regulatory standards applicable to those different classification might be a fact to recognize that could form a basis for future recommendations.

CHAIRMAN RYAN: Yes, and again, that's not unlike the effort that's on hiatus at the moment here in the U.S., the disposition of solid material activities. So I agree and I don't discount your point that there are some interesting schemes and in a particular country seem to offer some thoughts and things to think about but again the translation part gets a little tough.

MR. LIEBERMAN: Thank you.

CHAIRMAN RYAN: Okay. Than you. But again, we'll certainly consider those things as they come to our attention. In fact, the Committee in May visited Japan and had some rather detailed briefings from the National Safety Committee I believe it's called equivalent to the Commission and we have a trip report summarizing that information that's available to the public.

Yes. Next sir please.

MR. LOVINGER: I'm Todd Lovinger, the Executive Director of the Low-Level Waste Forum, and the Forum as most of you are probably aware, members of the Forum are comprised of the governors appointees for the states as well as the appointees from the compact commissions. At our meeting in September, the Forum passed a Discussion of Issues document. It is not intended to be a position statement, but it is intended to be an outline of this issue and to discuss both some of the benefits and drawbacks of the current system as well as what some of the benefits and drawbacks are to alternative approaches that have been discussed and recommended. I would encourage you to look at that also. We provided copies I know to both yourself and to Sharon.

CHAIRMAN RYAN: Great. We appreciate your mentioning that for the record and that again is a good forum of folks involved in this industry in this area and we appreciate you making that available to us. Thank you. Anything else at the moment?

MR. HAMDAN: Can I say something?

CHAIRMAN RYAN: Please Latif. Yes.

MR. HAMDAN: Just because all you have is two months and you want to submit this by December and I noticed that Part 3 is still blank. You haven't said anything about the recommendations. You may want to start thinking about the nature and scope of what the committee recommendations might be, what you might include and what you might not want to include early on so that it helps the process, the efficiency of finishing the report.

CHAIRMAN RYAN: I agree. Thank you. So we're going to work hard in the next month is what you're saying. Thanks for keeping us right on the center line, Latif. That's fabulous. I agree and I think once the committee digests the draft and we finalize the report, we'll be prepared at the December meeting to consider that kind of summary of issues and again, I don't think we'll necessarily offer solutions but perhaps identify issues, opportunities, challenges, that we see from this study and this analysis and from the other input that we get from other forums and so forth. Mike.

MR. LEE: This hasn't gone through any grammarian or technical editors. So what you see is --

CHAIRMAN RYAN: Any and all comments are welcome. No backing off, Mike.

MR. LEE: Nothing rhetorical.

CHAIRMAN RYAN: Again, I appreciate everybody's participation. This is a relatively short session. But in the interest of being fair and open and we wanted to get this out and get it on the record that we have this activity underway and we'll be reporting this out next month and to the Commission shortly thereafter, we welcome any and all input. Any other questions?

MR. FLACK: Just one more, Mike.

CHAIRMAN RYAN: Yes, please. John Flack.

MR. FLACK: This is John Flack, ACNW Staff. I guess from what I heard is that Part 61 is not broken. So then it must be in the implementation of Part 61 that the issue arises as to why we don't have access to these sites. So it would be in that context that the recommendations would be make. Is that right?

CHAIRMAN RYAN: No, I don't think that's necessarily so. I think there are lots of levels of issues. For example, and this is a very practical one, very small quantity sealed sources like strontium-90 eye application that eye doctors use and so forth, by calculation of the sources itself and again correct me if I'm wrong, Alan, can actually be "greater than Class C on a concentration basis" and there are other sources in that category.

But when you look at the absolute amount of radioactivity, it's trivial compared to what's disposed on a routine basis at a low-level waste site. So in certain states with certain licenses for facilities, those accommodations have been made for robust packaging for those sealed sources and they're deemed to be appropriate for low-level waste disposal. It's things of that sort that are kind of practical ones. That's a problem solved.

MR. FLACK: But you wouldn't have to go back to rulemaking to solve that problem.

CHAIRMAN RYAN: Again, I want to be very

careful here. I don't think we're even suggesting that at this point. We're studying the question. I don't know what will come out of it. This isn't a study aimed at supporting a position. This is a study of where things are.

So at this point, we're not at the step, at least, in my view of saying how you would fix something. Let's figure out what, if anything, is on the to-fix list and what might not be. So once we get that step done and have input and hear expressions and views on that aspect of it, then we can make the next step. But I think I want to be cautious and careful not to jump ahead to some solution that may or may not be appropriate, helpful or needed. So we're taking this in a careful step wise fashion.

Other questions or comments? With that, Alan, I think we will close this part of our meeting. We appreciate your participation from the other coast.

MR. PASTERNAK: Thank you very much.

CHAIRMAN RYAN: And we'll certainly take your suggestions carefully under advisement and look forward to your future participation.

MR. PASTERNAK: Thank you very much. I appreciate it.

CHAIRMAN RYAN: Thank you. Any other

questions or comments? With that, I think we'll close this part of the meeting and we'll get back to our letter writing. I appreciate everybody's attendance and participating and we'll close the record and go back to letter writing. Off the record.

(Whereupon, at 3:36 p.m., the above-entitled matter was concluded.)