

## HLWYM HEmails

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**From:** Christopher Grossman  
**Sent:** Thursday, February 22, 2007 3:42 PM  
**To:** Osvaldo Pensado  
**Cc:** James Winterle; Bret Leslie  
**Subject:** Fwd: Comment on TPA 5.1 and proposed work  
**Attachments:** tpa51beta\_comments.wpd

Osvaldo-

Attached are Dick's comments on CNWRA's approaches to resolving the 5 issues. In summary, he agreed on issues 1-3, but had some comments for Input Parameterization (mainly dealing with treatment of variability vs. uncertainty) that can be considered in finalizing input parameters for the code. Please see the attached for the details. I plan to talk with Dick later this week, so if you want to respond, please feel free or call Dick directly to discuss. I'll incorporate any feedback into my discussion with him later.

Thanks  
Chris

>>> Richard Codell <[richardcodell@yahoo.com](mailto:richardcodell@yahoo.com)> 02/22/2007 2:53 AM >>>  
Chris:

Here is my promised comments and suggested work on TPA 5.1. Consider this version a draft until you have a chance to review it and maybe pass it along to the NRC staff before we send the comments to the Center. Maybe some of my concerns can be addressed by a telecon between NRC and Center staffs that would create less waves among senior managers and less interruption to the current schedules.

Give me a call if you like. Call my cell [801-828-5269] if you can't reach me at home [(801) 572-5592].

Dick

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**From:** Christopher Grossman

**Created By:** Christopher.Grossman@nrc.gov

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2/19/07

Note to: Chris Grossman  
From: Dick Codell  
Subject: Comments on CNWRA TPA Approach of 1/24/2007 and recommended course of my work

I have several comments concerning the CNWRA proposal to address concerns with the TPA5.1 code finalization. I also want to tie-in some of my concerns with the projects suggested for me by Osvaldo. I also generated comments based on examination of the TPA input file and of the FORTRAN code. I will not cover all areas with equal rigor because it would spread my efforts too thin, so I will concentrate on a few areas.

#### Comments and questions

Issue 1 - "Rate of Inventory Release to the Geosphere" - The Center's memorandum Starting on page 3 discusses the technical basis for the rate of inventory release.

- a. Bathtub model - I agree that its appropriate to scrap the bathtub model in favor of the flow-through approach only. The bathtub model adds another layer of complication that physically probably doesn't make enough sense to keep in TPA. Also, eliminating the bathtub model and its fill-up time allows a considerable simplification and improved understanding of release model in terms of other, probably more important factors such as changes of infiltration rate and number of wetted waste packages with time.
- b. Diffusion model - I think there is ample reason to believe that diffusive release will be small compared to advective release. Even for cases where diffusion may be the largest release path, I believe it can be shown that (dose) consequences for those cases will be small. I have made such proofs myself over the years and have circulated them to the staff. The only case where diffusive releases approached advective releases was there is a pulverized source term intimately in contact with the rock, with no protection from any engineered barrier. Even for this case, the diffusion model in TPA would be inappropriate, since it was based on DOE's model of diffusion along a thin-film pathway inside the waste packages. I believe that Osvaldo's Task 2 can be relatively easily addressed.
- c. Cladding rupture model - Also referred to on Page 3. I think that its OK to scrap this model too. Simply assuming that the clad fails instantaneously rather than at a rate dictated by the swelling of spent fuel will be conservative. I wouldn't go as far as to say that the model lacks a sound technical basis. There is a considerable body of data from reactor operating experience and laboratory experiments on dry unzipping of hot fuel rods with leaking cladding. Its less likely that wet unzipping of cooler fuel would occur

however. The proposed model does not allow for an evolution of the failure of the cladding. I don't know how one would go about defending a model for this evolution however, so it probably leaves us little choice but to assume a stationary fuel exposure fraction that occurs instantly upon failure.

- d. Deletion of four time ranges for mechanical breach of the waste packages - I don't think the Center gives an adequate justification for deleting this provision. The four time ranges were an attempt to simulate a coarse distribution of failures in time, so that additional source terms for waste packages could be added as they failed. This is a reasonable goal, although it clearly introduces more complexity to the TPA code. Is the justification that the mechanical failures don't add that much dose to the calculation, and therefore all mechanical failures should be assumed conservatively to occur at the same time?

#### Issue 2 - Low Probability Seismic Event Sampling

I read over the October 11, 2006 presentation by Mancillas and Pensado. It looks like a good piece of work, and I agree with the conclusions that the undersampling is not likely to be very important to the final dose numbers.

#### Issue 4 - Input parameterization

I have long-standing problems with input parameterization in current versions of TPA.

##### Use of sampled parameter ranges that are probably not supported by any real data

Foremost of my concerns is the still-significant number of parameters specified in the input file that do nothing more than sample between a range for the purpose of expressing some sort of either (1) a random process or event, or (2) an uncertainty in a parameter. For example, the parameters like *SFWettedFraction\_SEISMO4\_9*, of which there are 40, don't appear to have any technical basis for their choice, and just add confusion to the results. We learn very little from this type of specification. It just adds noise to the interpretation. I am not even sure that the parameters are supposed to represent variability (aleatory) or uncertainty (epistemic).

##### A seemingly random chemistry for corrosion models

I see a potential problem with the environmental specifications for concentrations of the waste package environment, e.g., parameters like *EnvironmentII\_CO3\_Subarea\_9[mol/L]*. There are distributions for all ions specified once per subarea within a realization, with no correlations to most other parameters in that subarea, and no correlations to other subareas. Therefore it looks like they are sampling a different chemistry for each subarea within a given vector. Is there any justification for the assumption that the concentrations of ions are independent, and not correlated strongly within and among subareas? I think this question needs to be examined and the current approach justified. It should be made clear whether this approach is an expression of

aleatory variability or epistemic uncertainty.

#### A seemingly random sampling for rock degradation parameters

I don't understand why the input parameterization for rock degradation is sampled independently for each subarea without any correlation among subareas. For example, why is bulking factor sampled independently for each subarea? It seems to me that the bulking factor is more an intrinsic property of the rock, and therefore should be sampled once per realization for the entire repository. Is there a sound basis for this approach?

#### Lack of recognition of the ensemble nature of the source term for thousands of waste packages

The ensemble nature of the repository is probably not being well-represented by the choice of 10 subareas with one representative waste package per subarea. Since each subarea will have on the order of 1000 waste packages, it's the behavior of the ensemble of waste packages in the subarea that counts.

It appears that most if not all of the models for waste package and drip-shield failure are unaffected by spatial variability; i.e., since the model parameters are always sampled from the same distributions, with no mechanistic model for spatial variability within realizations, the failure of the engineered barrier components would be "statistically uniform" (also known as *ergodic*). If you repeated many realizations, I expect you would find that the distributions of failure times from all the causes (corrosion, drift collapse) would be ergodic. To the extent that I understand all the failure models in TPA, I don't see any mechanisms that impart any real spatial or temporal variability (i.e., aleatory) to the failure times. If the observation of statistical uniformity can be justified, then it would be better to do all the sampling of engineered barrier failures outside of TPA, and just pass along the resulting distribution to be used in the actual TPA calculations.

#### Recommendations for exploring the importance of ensemble treatment of the source term

I recognize that there has been a large investment in the current TPA code structure, and at this late date it might not be practical to develop the codes to do the failure calculations external to TPA. I examined the code modules for failure, and think it would take a considerable effort to perform such a re-programming. Nevertheless, I see two reasonable computational auxiliary analyses that would help us understand some of the issues with the treatment of the ensemble behavior of the source term:

1. Just by running the TPA code for a reasonably large set of realizations, and assuming that the failure times are statistically similar, then all realizations can be combined into a single population from which a failure-time distribution can be easily derived. If we have the failure time distribution derived from a large population available, then it can be used to estimate the potential errors we might be making by sampling only 10 representative waste packages per realization. What I expect this analysis will show is that the

variability of releases from the subareas will have a smaller variance than the 10-waste package result, resulting in fewer large dose realizations. How much smaller, I cannot yet judge. The importance of this result would be to diminish the upper (and lower) tail-end doses being calculated, but not as likely to change the mean dose as much. However, it is the infrequent realizations with large doses that often stand out in the results, and if the eventual HLW rule relies to some extent on the upper percentile doses, the effect of this calculation could be significant.

2. The current TPA code with 10 representative waste packages may underestimate the effects of nonlinear behavior such as solubility limits. Furthermore, the TPA code cannot address directly the problem of an increasing number of leaking or wetted waste packages over time in a given realization. I believe that this is partially addressed by having a time-dependent subarea wet fraction, but this is an approximation and doesn't actually allow changes in the number of active waste packages with time. Simply having a failure time distribution generated in the above step will not address this problem directly.

I have already embarked on a demonstration of the extent of this potential problem. I picked up where I left off from about a year ago, and feel strongly about performing this demonstration. Basically, the demonstration is structured on the comparison of the releases versus time for the entire repository either represented by 10 representative waste packages or 1000 individual waste packages, taking into account real spatial and temporal (aleatory) variability among the waste packages, and parameter sampling between realizations to represent epistemic uncertainty. The demonstration has the following features:

- a. It considers a single radionuclide, such as Np-237, which has a release rate from spent fuel that is either solubility limited or dissolution rate limited.
- b. No radioactive decay (very long half life).
- c. Nonlinear cutoff of release rate if solubility limit comes into play.
- d. Newly wetted and failed waste packages can be added as the subarea wet fraction increases with increasing time-dependent infiltration rate.
- e. No accounting of the effect of the flow path or of dose models.

I believe the above assumptions are justified, since it is known that Np-237 can be either solubility limited or dissolution rate limited, has a very high dose factor, has a very long half-life, and is abundant in spent fuel. This radionuclide also has a low retardation in the geosphere, so the effect of transport in the ground is probably not too important either.

I can't really see how to prove these points without such an experiment. For practical reasons, it is not possible to use the TPA code directly because of the extensive changes that would be needed, and the very long run times that would be necessary. Instead, the approach I am using is to extract a subset of the TPA 4.1 code, highly streamlined to minimize complications (like groundwater transport, other radionuclides, and dose models) in order to get a computer code

that can be run in a reasonable amount of computer time for this demonstration.

This demonstration will have two parts:

- (a) Demonstrate whether releases from the repository can be adequately represented by 10 subareas.
- (b) Demonstrate if a different input parameter distribution is needed or is possible to represent the ensemble.

### Conclusions and Recommendations

I have raised a number of concerns with the progress of necessary changes to the TPA code. I am requesting clarification from the Center developers on the parameterization of models within TPA and the treatment of (1) aleatory variability, (2) epistemic uncertainty, and (3) the treatment of the ensemble nature of the source term.

In terms of my own work on issues concerning TPA, I propose to work on several topics, in order of my priority:

Task 3 - Granularity/Ensemble averaging - I propose above to use the TPA 5.1 code to generate a distribution of failure times, and attempt to use this distribution to show how the correct treatment of the ensemble of waste packages might lead to smaller variance in reported doses. I also propose to use a separate model, highly abstracted from TPA 4.1, to demonstrate the effect of ensemble averaging and the importance of the number of active waste packages as they increase with time.

Task 1 - SFWettedFraction and correlation to seepage parameters - I propose to examine the assumptions being made in TPA 5.1 on the correlation among seepage factors. I will also look at the alternative approach of sampling the seepage parameters for each of the 10 subareas rather than once per realization, and how this might or might not be justified by information on spatial variability available for the site. I believe that I have a good feel for this topic because of my initial investigation of seepage models for earlier TPA models.

Task 2 - Diffusive release model - I already stated that I believe that this model can probably be eliminated based on several calculations of the relative unimportance of diffusion to the calculation of significant doses. I will search my notes on diffusive releases to further justify this position.