HLWYM HEmails

From: Bret Leslie
Sent: Wednesday, March 07, 2007 2:10 PM
To: James Winterle; Christopher Grossman
Cc: Chandrika Manepally; David Pickett; James Myers; James Durham; Luis Ibarra; Osvaldo Pensado; Bret Leslie; David Brooks; Mysore Nataraja; Randall Fedors; Tae Ahn
Subject: RE: comments on SVTP attached and useful language for user guide chapters
Attachments: CodellQuestionsResponses.wpd

Jim,
Thanks for addressing my comments and for providing Osvaldo's cogent (even for this geochemist) explanation of the treatment of variability within the general "near-field area" in the TPA code. It is a good system-level perspective.

the information used to respond to dick's general question 2-4 in the attached file, is well suited for the model support sections of the NFENV, EBSFAIL, MECHFAIL, and EBSREL user guide chapters. the goal of the model support section of the user guide is to provide some understanding for why the particular approach used is appropriate. The thoughts contained in Osvaldo's explanation for the approach should be considered for inclusion in the above identified chapters. (Osvaldo - thanks again for making things clearer)
bret

>>> James Winterle <jwinterle@cnwra.swri.edu> 03/07/2007 12:25 PM >>>
Chris, Bret:

Thanks for the helpful comments. I incorporated the suggested changes and the revised version will be on the shared drive shortly. I still have to address any QA or programmatic comments,which should be done by the end of the week, before it is final. There were some questions in Bret's comments that I try to address below. Let me know if there are additional questions. Chris, note also that I made some changes to the text for tasks S-2 and S-4; since you wrote those originally, I hope you can take a look to make sure the changes are OK. Especially look at the caveats I added to the description of S-4.

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Comment responses:

Comment for section 6.1.9: "*Is there variability in chemistry or is there variability in subareas' chemistry (chemistry of subarea 1 different than subarea 7). If the latter what is the basis for this? In any realization is only one chemistry chosen for all or subareas or is chemistry sampled for each subarea?*
Response: Chemistry if variable for each subarea. **The reason why is pehaps best addressed in the recent reply by Osvaldo to similar questions from Dick Codell; see response to questions 2-4 in the attached file.**

Comment on section 6.1.11: *Does this imply that U is a colloid? Why are the 3 elements in this **sentence** different than the four specified as colloids?*
Response: The sentence refers to **reversible** colloid sorption, whereas the four elements referred to in the previous section are related are the species that form intrinsic colloids or irreversibly sorb to colloids.

-----Original Message-----
From: Christopher Grossman [mailto:CJG2@nrc.gov]
Sent: Tuesday, March 06, 2007 4:39 PM
To: Jim Winterle
Cc: Bret Leslie
Subject: Fwd: comments on SVTP attached (in italics) EOM

Jim-

Bret provided comments on the SVTP. Please address as appropriate. We can discuss in our Thursday call.

Bret-

In response to your question on task S-2: Radionuclide Release Rates, the difference is the first bullet is at a scale of the single waste package. The second bullet broadens out to a single subarea with multiple waste packages. The third bullet expands even further to the entire repository. Let me know if you have any further questions.

Chris

>>> Bret Leslie 03/06/2007 9:19 AM >>>
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Created By: Bret.Leslie@nrc.gov

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Question 1:

> 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?

Response:
The new model for seismicity, incorporated into MECHFAIL, only outputs two arbitrary failure times and the fraction of WPs affected at those times for each subarea. These two times are actually used in RELEASET, as opposed to being mapped into time intervals as done in TPA 4.0 (?). The new MECHFAIL abstraction heavily relies on the "representative WP" concept. Because the model is designed to track only two representative WPs in a subarea, only two breach times are reported. Alternative models could have been developed, but MECHFAIL was designed consistent with the global TPA code philosophy of considering one or few representative WPs per subarea. With respect to the justification on whether this approach is reasonable or finer discretization should have been pursued; this is an open question applicable in many components of the TPA code. Similar questions exist in the appropriate level of discretization for the selection of "representative" flow rates, chemistry, waste package breaching, source term, and so on. We need additional work to try to address this discretization question in general. The approach proposed by Codell for "ensemble treatment of the source term" is a good starting point probably extendable to MECHFAIL.

Additional comments of the four seismic ranges. In the past we considered the following WP breaching classes

1) Initially defective
2) WP corrosion
3) Faulting
4) Seismic
5) Seismic (4 different time intervals, referred to Seismic 1, 2, 3, and 4)

Thus RELEASET allowed us to consider up to 8 WP sources inserted in the system at 8 different times. The new WP breach classes are

1) Initially defective
2) General corrosion
3) Faulting
4) MECH 1 and MECH 2 (two different rock types)
5) Localized corrosion

Incorporation of the revised MECHFAIL rendered Seismic 3 and 4 as free classes. There is a need to consider up to 7 WP sources in RELEASET. We have strived to minimize changes to RELEASET. Accordingly, we used Seismic 1 and Seismic 2 to incorporate MECH 1 and MECH 2 (representing lithophysal and non-lithophysal regions) and Seismic 4 to incorporate localized corrosion waste packages. Seismic 3 is still free to be used. Therefore, the old Seismic 1, 2, 3, and 4 have lost their meaning, and it is recommended to remove the associated 4-time intervals from the tpa.inp file (as those intervals are not activated anymore by the TPA code).

Question 2

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).

Question 3

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.

Question 4

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?

Response to Questions 2 – 4

We will try to respond together to these questions as they are three expressions of the same issue.

The split into N subareas was originally intended to capture variability in the deep percolation and stratigraphy. The desire was that any subarea dependent parameter was associated to a feature of the subarea, and parameters not correlated to a subarea would be sampled once per realization.

The first parameter breaking that requirement was the SFWettedFraction, which was sampled per subarea and failure mode. The origin of this decision is not clear now, but the approach is not necessarily unreasonable as next explained.

Next to the requirement that the TPA could should capture subarea variability was the requirement that each TPA realization should yield meaningful results, and possibly represent a "likely" future. This later requirement is inconsistent with requesting a single sample per realization for parameters that are not subarea dependent. For example

i) It is not reasonable that all of the WPs breached in the repository fill up to 30% of the internal volume (the fill up volume is controlled by SFWettedFraction)

ii) It is not reasonable that all of the WPs in the repository are subject to water with pH=5 and

experience localized corrosion

iii) It is not reasonable a sharp contact angle between the DS and the WP causing all of the WPs in the repository to breach

Such cases arise if requested that non-subarea parameters are sampled once per realization. The single-sample requirement leads to extreme realizations where all of the WPs fail, with high flow rates, low retardation, fast transport, and unrealistically high doses. Thus, the single-sample-per-realization requirement is inconsistent with the requirement that results from independent realizations make sense.

Now it is clear that several layers of discretization are needed in the design of a performance assessment model. A discretization layer could be aimed at capturing variations in the thermal-hydrology, another at variations in the stratigraphy, another at changes in rock properties (e.g., lithophysal and non-lithophysal). Finer discretization layers could be aimed at capturing smaller scale aleatory variability (e.g., water chemistry may vary from seepage point to seepage point; corrosion rates could vary not only from waste package to waste package but even within a single waste package). All of these multiple discretization layers are not available in the TPA code (it is not practical). As a gross approximation, we adopted the subarea discretization for the various required discretization layers.

For example, in the water chemistry, 10 different water compositions are considered in a single realization. This variability is aimed at capturing stochastic variability. After multiple realizations, there is no bias in the average number of waste packages affected by localized corrosion (any subarea is as likely to exhibit localized corrosion). The approach may still overestimate the variance in the number of localized corrosion breached waste packages, as not all of the physical stochastic variability is yet captured (e.g., corrosion rates may also exhibit package to package fluctuations). However, the variance is smaller than the one resulting from assuming that the water chemistry be the same throughout the repository.

Therefore, the subarea discretization is used to fulfill two purposes. On one hand it captures the deep percolation and stratigraphy variation; on the other, it is used to allow for stochastic variability in the system. We judged convenient to allow for variability in relevant parameters linked to mechanical breaching and localized corrosion breaching of the waste package. Again, such variability is aleatory, not connected to subarea definitions. We could enforce the single-sample-per-realization requirement at the cost of deriving single realization outputs with non-reasonable results. In this approach, the only meaningful output would be statistics of multiple realization data. Also, since variances would be grossly overestimated, more realizations would be needed to reach convergence. On the other hand, in our proposed approach, more converging statistics are derived with a smaller number of realizations.

Specific comments for Questions 2 – 4
Question 2
With respect to SFWettedFraction, the proposal is to have SFWettedFraction_LC_X = loguniform(0.007, 0.156) correlated to InitialSeepageReductionFractionLC = loguniform(0.001, 0.1), with a correlation coefficient of 0.9. The rationale is that the SFWettedFraction should correlate with the size of the opening on the WP (size related to the parameter InitialSeepageReductionFraction). The range of the parameter SFWettedFraction_LC_X is selected to force the fraction of the exposed waste form surface range from 0.001 to 0.1. The exposed waste form surface is assumed to vary similarly as the parameter InitialSeepageReductionFraction.

Likewise, SFWettedFraction_Initial_X=loguniform(0.007, 0.156) is prosed correlated to InitialSeepageReductionFractionLC = loguniform(0.001, 0.1) with a correlation coefficient of 0.9.

The parameters SFWettedFraction_SEISMO1_X and SFWettedFraction_SEISMO2_X are assumed uniform(0.033, 1.0) (range selected to force the fraction of the exposed waste form surface range from 0.01 to 1.0). These parameters will be correlated to InitialSeepageReductionFractionByMechFailedW = uniform(0.01, 1.0) with a 0.9 rank correlation coefficient.

Sampling of the SFWettedFraction per subarea causes variability in the spent fuel dissolution rate. Having subarea to subarea variability in this parameter causes less extreme radionuclide releases for those realizations having all of the WPs breached.

Question 3
The main reason of the selection of sampling per subarea is to have a smoother distribution of WP breaching by localized corrosion. Only the Environmental parameters are sampled per subarea.

Question 4
The use of one bulking factor implies perfect correlation among all the subareas. The bulking factor at each subarea, however, depends on several rock characteristics, as mentioned in the question. Then, the use of one bulking factor is not the best approach.

In an ideal situation, a probabilistic distribution function (PDF) should be obtained for the bulking factor for each one of the two rock types discretized at each subarea. Note that to avoid different rock types in each subarea, the subareas should have been divided according to differences in rock characterization, which is not the case.

Probably, the next best alternative is to group the rock data according to major differences such as lithophysal and non-lithophysal rock, independently of the subarea in which the rock is located. Then, obtain PDFs for the bulking factors for these two cases and sample bulking factors for each type of rock at each subarea, according to these PDFs. This is a way to roughly account for spatial variability, but requires rock characterizations for all the subareas and studies to obtain bulking factor PDFs.

Randomly selecting from one big area or ten subareas will not appreciably modify the outcome if enough number of realizations are performed, unless the rock characteristics for each subarea are different. The is not the current approach because each bulking factor is sampled for each type of rock at each subarea using the same probabilistic distribution. Thus, until this rock characterization is done, the only advantages of the current method are that (1) less realizations are needed to reach stable results and (2) the program has the flexibility to incorporate any new rock data obtained from site studies.