HLWYM HEmails

From: Bret Leslie
Sent: Wednesday, August 24, 2005 2:54 PM
To: James Winterle; Bret Leslie
Cc: Sitakanta Mohanty; Andy Campbell; Christopher Grossman; Deborah DeMarco
Subject: Re: ACTION: Please review and implement deliverable guidance
Attachments: TPA 5.01 Development Issues_08_24_05.doc; TPA 5.0.1 action items.doc; tpa guidance.doc

Jim,
Find updated action list for TPA 5.0.1 attached (TPA 5.01 Development Issues_08_24_05.doc). This reflects all the action items for all presentations to date. The updated ones are on seepage and "MECHFAIL." As per my Email of 08/08/05 5:49 PM (below, and attached files) please address the action items in milestone report.
thanks for your assistance,
Bret

>>> Bret Leslie 08/08/05 5:49 PM >>>
Jim,
Attached find guidance for a deliverable and a list of actions items for the TPA code that are identified in the guidance document. The ideas identified in the guidance were discussed with you and Andy last Friday and we agreed to codify the guidance in writing.

Together we must continue to work to ensure development of the TPA code is integrated at the center and is integrated and developed jointly with the NRC. This may require for both of us to think of ways to accomplish this both in terms of program directions (operations plan) and in practice (e.g. discussion of issues before implementation or settling on values for parameters). If you have any question please don't heistate to contact me.
Bret Leslie, Program Element Manager MOSP

Bret W. Leslie, Ph.D.
U.S. Nuclear Regulatory Commission
MS T-7F27
Washington, DC 20555-0001
(301) 415-6652
FAX 301 415-5398
bwl@nrc.gov

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Subject: Re: ACTION: Please review and implement deliverable guidance
Sent Date: 8/24/2005 2:54:07 PM
Received Date: 8/24/2005 2:54:43 PM
From: Bret Leslie

Created By: Bret.Leslie@nrc.gov

Recipients:
"Sitakanta Mohanty" <smohanty@cnwra.swri.edu>
Tracking Status: None
"Andy Campbell" <Andy.Campbell@nrc.gov>
Tracking Status: None
"Christopher Grossman" <Christopher.Grossman@nrc.gov>
Tracking Status: None
"Deborah DeMarco" <Deborah.DeMarco@nrc.gov>
Tracking Status: None
"James Winterle" <jwinterle@cnwra.swri.edu>
Tracking Status: None
"Bret Leslie" <Bret.Leslie@nrc.gov>
Tracking Status: None

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Files	**Size**	**Date & Time**
MESSAGE	1311	8/24/2005 2:54:43 PM
TPA 5.01 Development Issues_08_24_05.doc	33345	
TPA 5.0.1 action items.doc	31808	
tpa guidance.doc	31296	

Options
Priority: Standard
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Reply Requested: No
Sensitivity: Normal
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Recipients Received:

TPA Action Items

Given the scope of the changes in TPA 5.0.1, a software requirements description probably should have been generated. The following issues have been identified as a result of presentations (A-E), on the basis for the TPA 5.0.1 code, by Center staff. Many of these issues relate to the conceptual models and the choice of parameters used in the TPA 5.0.1 abstractions. These issues have been identified during the model validation process, but should have been identified, addressed, and discussed during development of the models prior to implementation in, and validation of, the TPA 5.0.1 code. Additional issues have been identified as the result of discussions between NRC staff and the Center staff. These issues need to be addressed, either in subsequent discussions, or in changes in the code, by the Center prior to release of a new version of the TPA code.

A. Colloids:

1. Address the assumption that all corrosion products (iron-bearing) are mobile. Corrosion products could accumulate within the waste package and may not all be “flushed out” of the waste package. There is evidence for large amounts of the actinides being left behind on the solid substrates in Ebert and Bates,1992, and in Finn et al., 1996 MRS paper, and in the acid strip test at PNNL.
2. The choice of sorptive iron-bearing phases, given the timing of degradation or iron-bearing components and stability of the different iron-bearing corrosion product phases, and the timing of release of radionulcides from spent fuel degradation, should be addressed.
3. Address whether the Cm-Am-Np chain can be incorporated, as the decay in-growth of Np, into the initial Np inventory. This could require that staff justify this assumption based on decay half lives, expected behavior of waste package degradation (time frame relative to half life of nuclides), and understanding of the risk significance of this decay chain (a small fraction of initial Np inventory).
4. Address the potential for overestimation of irreversible colloid release and transport because waste form particles and intrinsic colloids (Pu) maybe unstable in farther field chemistries.
5. If not part of the validation studies completed, demonstrate that mass is conserved.
6. Address whether physical filtration in the invert, which is currently set to zero, is realistic. If it is determined that the current approach is unrealistic, and a technical basis for a more realistic approach can be developed, then implement a more realistic approach.

B. Corrosion of Waste Package and Drip Shield and the Near Field Geochemical Environment

1. Identify those variables in the tpa.inp that should not be changed individually (e.g. the passive current density is linked to the corrosion potential).
2. Address whether the failure criterion for Alloy-22 accounts for a non-homogeneous roughness or requires the full thickness to be penetrated before it is considered to be failed.
3. Address whether physical separation of the drip shield will impact the percentage of waste packages affected by adverse fluid compositions.
4. Address whether all the important uncertainties, including features, events and processes, have been captured in the current conceptualization.
5. Address whether strengthening the technical basis or revising parameters to account for range of general corrosion rates considering effect on localized corrosion and DOE's data is required.
6. Address whether and how a technical basis for extrapolating data above 95degC can be generated.

C. Subareas

1. Address whether the subareas adequately depict the thermal regime, its variability (e.g., different conductivities of units and edge cooling effects could lead to widely variable temperature and humidity time histories for a single subarea), and its impact on corrosion and radionuclide release.
2. Address whether the subareas adequately depict the mechanical degradation, its variability (e.g., lithophysal and non-lithophysal units may have very different drift degradation characteristics and a single subarea may contain more than one rock unit), and its impact on corrosion and radionuclide release.
3. Address whether subarea 3 needs to be split because of its large area, and its consequent large percentage (~60%) of inventory. Take into account items one and two above in determining whether and how this subarea could be divided.
4. Address how the four seismic modes are addressed for the subareas and whether the values of parameters which are subarea-specific in tpa.inp (e.g., SFWettedFraction_SEISMO1_#) need to be changed as the result of the new subareas in TPA 5.0.1, and address whether their values are consistent with the flow model for the waste package (bathtub versus flow through).
5. Remove subarea coordinates from tpa.inp and place into a data file.
6. Review tpa.inp to determine which items should not be in the file, but should be considered for placement in data files.

D. Non-Colloidal Radionuclide Transport in Unsaturated and Saturated Zone

1. Address Cm issue (see item #3 of colloids above).
2. Address the issue of modifying pH and P_{CO2} (see #6 in subareas) in tpa.inp when modifying their range could result in non-desired results (default Ka is 0).
3. Address NEFTRAN and unit interface issue.

E. Redistribution and Mass Loading Associated with the Igneous Extrusive Scenario

1. Abstraction should be consistent with 10 CFR 63 concept of the reasonably maximally exposed individual and not presume the location of the individual in, or directly adjacent to, the depositional fan of Forty Mile Wash.
2. Address the apparent disconnect of ASHREMBO from VOLCANO. Consider re-scaling TEPHRA runs to a single waste package and then use that to extrapolate for the number of waste package damaged, as determined by VOLCANO. Identify what other parameters from VOLCANO will need to be considered for consistency.
3. Address the basis for only including inhalation dose estimates for ASHREMOB.
4. Address the need for a strengthened technical basis or revised conceptual model to address for the lack of decay related to fluvial remobilization.
5. Address, or otherwise develop, a technical basis for the three weighting factors (initial, fluvial, and eolian).

F. Revised standard

1. In the SRD a placeholder should identify that any changes in the TPA code necessary to address specific regulatory requirements would be addressed.

G. Drift Degradation and Mechanical Degradation of Engineered Barrier System

1. Address, or strengthen, technical basis for timing and the uncertainty of drift degradation

input parameters. Evaluate the importance of timing assumption on near-field environment. Also, consider conditions relevant to Yucca Mountain, including geology and thermal characteristics, when evaluating model support analogs. For instance, is there information in silver mines, Hoover Dam tunnels, etc.
2. The current model assumes the waste package fails if the outer package is breached, mechanically or chemically. Address, or account for, conservatisms in waste package failure mode assumptions, particularly for the drift degradation scenario.
3. Ensure waste package failure mode concepts are consistent with flow modeling concepts (e.g., flow factor adjustments, default water contact mode, etc.). Address, or develop, technical basis for integration of abstractions.
4. Provide an understanding of impact of mechanical failures and bulking factors for all subareas. Address consistency/discrepancy between subareas. Address appropriateness of rock types and lithology for subareas.
5. Address the impact of intact lithophysal void space (5-30%) on quantity of mass of rock degraded.

H. Seepage
1. Ensure TPA provides for sufficient *.res files to interpret results and understand output of consequence modules (e.g., ASHREMOB). In the SRD, identify areas where additional *.res files should be added as well as areas that no longer require *.res files because of modeling changes, etc.
2. Data in the file infilper.res was identified as confusing from understanding of older code versions. Ensure data in output files is appropriately calculated and categorized, and is consistent with current understanding.
3. Continue evaluating implications of representing many source terms by a small number of representative source terms.
4. Ensure flow modeling (e.g., dryout thickness input files and along-wall flow conceptual model) is consistent for all included scenarios (e.g., drift degradation).
5. Address, or otherwise develop, a technical basis for the changes the TPA code leading to reductions in uncertainty for flow modeling.
6. Address, or otherwise develop, a technical basis for the default contact mode of water and the waste form.
7. Ensure reflux models are consistent with thermal time histories and time frames established by regulatory requirements.
8. Address program costs and benefits (e.g., risk significance) of potential modifications.

Potential Action Items to be identified on the following topics.
I. Climate and Infiltration

TPA Action Items

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Potential Action Items to be identified on the following topics.

August 8, 2005

G. Drift Degradation and Mechanical Degradation of Engineered Barrier System
H. Seepage
I. Climate and Infiltration

August 8, 2005

Guidance for CNWRA Milestone 06002.01.354.520

Introduction

This milestone, originally due on July 25, 2005, has been delayed once to September 16, 2005, with no change in scope. This guidance, presented below, changes both the scope and date of the deliverable to September 30, 2005. The title of the original milestone was "Validated Fortran Source Code for TPA Version 5.0.1." The NRC's intent for the milestone was to deliver a version of the TPA code that could be used, in a defensible manner, during the review of a potential license application, which in January 2005, was expected to be submitted in late 2005. The objective was, and remains, to provide a technically defensible, and validated, version of the code, several months prior to a license application, which is now expected no sooner than March 2006. Thus the schedule for delivery of a technically defensible, in terms of model validation and justification of model parameters, and validated version of the code should be reflective of the date of submission of a potential license application.

Background and Analysis

At the Center, Technical Operating Procedure #18 (TOP-18) guides development of, and controls use of, software. Previous versions of TOP-018 had included model validation as part of the procedure. Thus NRC had assumed, when requesting a validated version of the code, that the models reflected in the code would be validated, to the extent possible. A new version of TOP-018, in December of 2004, changed this approach and only mentions model validation in the definitions section of the procedure. The new version of TOP-018 (December 2004) focuses solely on software validation and controlled development of TPA version 5.0.1 deliverable.

As early as January 2005 it appears that the NRC and Center were holding different expectations for the TPA code deliverable. For instance, on January 21, 2005, in response to a January 19 presentation to the Yucca Team on the expectations for the development and use of the code, Wes Patrick sent an email to the NRC on clarification on software validation. In the note he states, "Model validation is a separate matter, per TOP-018 and as the term is generally used in the profession. TOP-018 defines model validation as the 'process of assuring that a mathematical model as embodied in a computer code (software) is an adequate representation of the process or phenomenon for the purpose for which it is intended.' ... The TOP-018 definition of model validation is consistent with that provided in NUREG-0856, which it cites. Namely, 'assurance that a model as embodied in a computer code is a correct representation of the process or system for which it is intended.' [Note that 'correct' was replaced with 'adequate' in TOP-018 to avoid any implication that NRC requires a valid model to be absolutely accurate. A model needs only to be adequate or sufficient for regulatory purposes.] Its clear aim is to test and assure that the actual model—the mathematical representation of the real-world process or system—reasonably/adequately represents that real-world process or system. This is a much different and higher standard that is NOT addressed in the software validation that is planned for the TPA code in the near-term schedule laid out in the YM Team meeting."

Unfortunately neither the NRC nor Center pursued this last sentence in the above quote, as it goes to the heart of the differing expectations for the deliverable. The NRC's requirements for an updated version of the TPA code were, and are, that models incorporated into the code reasonably represent the real-world processes, are consistent with the regulatory framework embodied in 10 CFR 63, and retain the flexibility necessary to evaluate a potential license application. The Center focused its efforts to meet its quality assurance requirements embodied in TOP-018. Nevertheless, substantial and meaningful progress has been achieved.

Status of Work

The Center and NRC staff have worked on providing values, and their justifications, for parameters in TPA 5.0.1. Substantial work, completed and in progress, at the Center on generating values for parameters and their justification, and process-level models and their abstractions, has been, or is being, documented in Center milestone reports in multiple program elements. Currently approximately one third of the over 1100 parameter values are missing their corresponding justifications. Substantial work has taken place on software validation of the TPA 5.0.1 code. As a result of NRC staff testing of beta versions of TPA 5.0.1 during validation of the TPA 5.0.1 code, several issues were identified for further discussion. The Center staff is providing a series of presentations on the identified areas of the code. So far, presentations on colloids, corrosion and near-field chemical environments, subareas, non-colloidal radionuclide transport in the unsaturated and saturated zone, and ash remobilization have been delivered. As a result of these presentations the NRC staff has identified a series of action items that need to be addressed. Additional presentations on drift degradation and its impacts on engineered barrier system, seepage, and climate and infiltration are expected to be delivered for discussion by the end of August. Additional action items are likely to result from these discussions.

Guidance

1. The date of the revised milestone is September 30, 2005, and this should be noted in the next Periodic Manager's Progress Report (PMPR) in the appropriate table.

2. The title of the milestone should be changed to reflect the scope of the deliverable and the items enumerated below.

3. The deliverable should include a software requirements description (SRD in TOP-018). The SRD should be for version 5.1, or other version as appropriate with respect to TOP-018. The SRD is to document the current TPA 5.0.1 approaches. The SRD should also identify the changes necessary to address NRC concerns on the technical acceptability of the current approaches in TPA 5.0.1 (these are the action items described above and the action items are enumerated in a separate file titled "TPA 5.0.1 action items").

4. The Center should stop the current software validation efforts on TPA 5.0.1 and focus the resources on development of SRD and addressing the action items.

5. The SRD will need to reflect the list of action items, which will be updated as the remaining presentations are given to NRC.

6. The deliverable or cover letter should identify the status of parameters and justification. Separately, and immediately, the list or parameters that still require justification, with the responsible individual identified, should be provided to the NRC program element manager.

7. The deliverable or cover letter should identify the presentations that have been provided to date, and how they have been given in a form that could support development of TPA manual.

8. The deliverable or cover letter should summarize the validation effort and identify what tasks that were completed in the validation of 5.0.1 that will need to be revisited for 5.1 (based upon the SRD that is developed).

9. The deliverable or cover letter should identify other FY05 CNWRA deliverables supporting the TPA development, both parameter (e.g., Radionuclide Transport, Unsaturated Zone Flow) and process level (e.g., redistribution, MECHFAIL).