HLWYM HEmails

From: James Mancillas
Sent: Wednesday, December 12, 2007 9:47 AM
To: David Pickett; James Prikryl; Osvaldo Pensado; Scott Painter; Xihua He; Yi-Ming Pan; Hakan Basagaoglu; Andy Jung
Cc: Christopher Markley; Keith Compton; Osvaldo Pensado
Subject: RE: ENG4 workshop on TSPA-SEIS abstractions
Attachments: TSPA_camp_ENG4.ppt

Follow Up Flag: Follow up
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All,

We will be holding a series of workshops on the TSPA-SEIS in the upcoming weeks. The objective of these workshops is to prepare Center and NRC staffs for a TSPA tech exchange with the DOE.

Through Keith Compton's efforts, workshops have been scheduled throughout the next few weeks, with a workshop focusing on each of the ISIs. The workshop for ENG4 is scheduled for December 19.

Key outcomes of these workshops are to:
(1) Identify key areas of concern within the TSPA modeling abstractions which we can address in a TSPA tech exchange.
(2) Identify intermediate results which will be needed for an acceptance review, but are not currently accessible/available to us (which we may be able address in a TSPA tech exchange).
(3) Identify intermediate results which may be sensitive to the treatment of parameter uncertainty.
(4) Staff to become familiar with the TSPA-SEIS model (which may be similar to the upcoming TSPA-LA).

A tentative agenda for the ENG4 meeting 8:30 -10:30: Discuss model description, model implementation,
: Break
1045 - 1200: Barrier capability analysis (as applicable)
: Lunch
1315 - 1415: FEP inclusion and implementation
1415 - 1500: Treatment of parameter and model uncertainty
: Break
1515 - 1630: Model Support, Data and Model Traceability, documentation of Q status

I expect that the bulk of the heavy lifting will occur during the morning, with the schedule being flexible and adaptable to discussions which occur during the first session.

To prepare for this workshop, I have developed a quick review of the topics covered by ENG4 within the TSPA. I ask that you skim through this review, and prepare by spending a few minutes refreshing you memory about:
--The model abstractions and flow of information --The documents needed to support your area of expertise --The parameter uncertainty used in the abstractions

Thank you

James Mancillas

-----Original Message-----
From: David Pickett [mailto:dpickett@cnwra.swri.edu]
Sent: Tuesday, December 11, 2007 1:17 PM

To: 'James Prikryl'; 'Osvaldo Pensado'; 'Scott Painter'; 'Xihua He'; 'Yi-ming Pan'; Hakan Basagaoglu; Hundal "Andy "Jung; James Mancillas
Subject: ENG4 workshop on TSPA-SEIS abstractions

ENG4 team,

On Wednesday, December 19, here at the Center, James Mancillas and Chris Markley will conduct a workshop on ENG4-relevant aspects of TSPA-SEIS.
I wouldn't expect all team members to attend the entire all-day session, but be looking for an agenda in case you want to hear about specific models. More info to come.

David

Hearing Identifier: HLW_YuccaMountain_Hold_EX
Email Number: 725

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Subject: RE: ENG4 workshop on TSPA-SEIS abstractions
Sent Date: 12/12/2007 9:47:04 AM
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From: James Mancillas

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ENG4

TSPA-SEIS Campaign

James Mancillas

Outline

- Present a quick review of ENG4 subject matter contained within TSPA-SEIS (Waste form degradation, EBS transport).

- Briefly explore relevant portions of the TSPA-SEIS model (a live exercise).
- Identify questions for DOE TSPA Tech exchange, and identify results and intermediate outputs necessary for an acceptance review.
- Identify areas in the model abstraction that are especially sensitive which should be given special attention during a review.

Review of Waste Form Degradation and Mobilization Model

Consists of Five Submodels

(1) Initial Radionuclide Inventory Submodel:

Defines the radionuclide inventory and radionuclides of importance

(2) In-Package Chemistry Submodel:

Evaluates in-package chemical conditions (vapor influx, seepage influx)

(3) Waste Form Degradation Rate Submodel:

Calculates the degradation rates of CSNF, DSNF and HLW

(4) Solubility Submodel:

Calculates solubilities of RN elements in a failed WP and in the invert

(5) EBS Colloids Submodel:

Calculates colloidal concentrations of RN in failed WP and in the invert

Analyses and Report Inputs

- *Initial Radionuclides Inventories* (SNL 2007 [DIRS 180472]) and *Radionuclides Screening* (SNL 2007 [DIRS 177424]).
- *In-Package Chemistry Abstraction* (SNL 2007 [DIRS 180506]).
- *CSNF Waste Form Degradation: Summary Abstraction* (BSC 2004 [DIRS 169987]), and *Other Waste Form Degradation Abstraction* (BSC 2004 [DIRS 172453]) and *Defense HLW Glass Degradation Model* (BSC 2004 [DIRS 169988]).
- *Dissolved Concentration Limits of Elements with Radioactive Isotopes* (SNL 2007 [DIRS 177418]).
- *Waste Form and In-Drift Colloids-Associated Radionuclide Concentrations: Abstraction and Summary* (SNL 2007 [DIRS177423]).

Key inputs into the Waste Form Degradation and Mobilization Model

- Set of initial materials within the WP and the materials' major elemental compositions and physical and chemical properties.
- Time-dependent water flux into a failed WP, provided by the *EBS Flow Submodel.*
- Temperature and relative humidity in the WP, provided by the *EBS TH Environment Submodel.*
- Partial pressure of CO2, provided by the *EBS Chemical Environment Submodel.*

- A key note

  The EBS Transport Submodel is implemented in the TSPA-SEIS at the scale of a single WP. The pertinent EBS Transport Submodel properties for a single representative WP are scaled to the total number of WOs that have failed in each percolation subregion. These properties include the mass of available inventory, pore water volumes, mass of solid materials, advective flow rates and diffusion areas

Model Abstractions

- Initial inventory (6.3.7.1)

  TSPA-SEIS initial inventory is used to assess the dose risk from 32 RNs, with 27 RN modeled explicitly (6.3.7.1.2). The initial mass of each RN, for each WP fuel type, is adjusted to account for the inventory distribution at the time repository closure. For each TSPA realization the initial masses are also adjusted to account for uncertainty in the source inventory by applying a multiplier (for each waste form CSNF, HLW glass and DSNF). The multiplier is sampled from a uniform distribution for CSNF [0.85,1.4], a triangular distribution for DSNF [0.45, 0.62, 2.9] and a triangular distribution [0.7, 1.0, 1.5] for HLW.

  From this initial inventory RN release can occur from the source both immediately (readily soluble RNs in the gap) and through the waste form degradation (RNs bound in the waste form matrix).

Model Abstractions

- In-Package Chemistry (6.3.7.2)

  The abstractions for determining the chemical parameters inside a failed WP are described in In-Package Chemistry Abstraction (SNL 2007 [DIRS 180506]). The submodel implements the evolution of the water chemistry inside a failed WP as a function of RH (EBS TH submodel), Pco_2 (EBS Chemical Environment submodel) and the water inflow rate (EBS Flow Submodel). The water chemistry determined in the In-package submodel is used by four other *Waste form Degradation and Mobilization* submodels. Specifically, the waste form matrix degradation rate for CSNF requires pH and Σco_3; the waste form matrix degradation rate for HLW requires pH; the dissolved concentration limits of radioactive elements require pH and ionic strength; and the stability of colloids requires pH and ionic strength.

  The In-Package Chemistry Abstractions are derived from the output of the In-Package Chemistry Process Models (SNL [DIRS 180506]) and provide either parameter distributions or response surfaces for the TSPA-SEIS.

The abstraction for the In-package chemistry Submodel consists of five parts

1. Determination of whether In-Package Chemistry needs to be calculated.

   No evaluation for low RH or inflows lass than 0.1 L/yr

2. Determination of which abstraction to be used.

   Ionic strength calculated using vapor flux (clean water) or liquid flux

3. Calculation of ionic strength.
4. Calculation of pH

   pH functions of CO2 and log ionic strength and influx flow

5. Calculation of the total concentration of aqueous carbonate.

   Total carbonate is a function of temperature, pH and Pco_2 and is based on equilibrium mass action expressions

Model Abstractions

- Waste Form Degradation(6.3.7.4)

  CSNF Waste Form Degradation Abstraction is described in *CSNF Waste Degradation: Summary Abstraction* (BSC 2004 [DIRS 169987]). The DSNF Waste form abstraction is described in DSNF and Other Waste Form Degradation Abstraction (BSC 2004 [DIRS 172453]). The abstracted models for the waste form matrix estimate the rates at which the CSNF and HLW waste forms degrade as a function of chemical conditions in failed WPs. For DSNF waste forms, an instant degradation rate in implemented, which is an upper limit degradation rate which is applied to all but naval SNF.

  For CSNF RN are released by (1) instantaneous release of the gap fraction inventory and (2) matrix dissolution under alkaline or acidic conditions. (Cesium, iodine, technetium and strontium are in the instantaneous release inventory.) Thus three inventories are considered: (1) hardware inventory (C14), (2) instantaneous release inventory, which is the fraction of the per-package inventory that is in the gap and grain boundaries, and (3) is the inventory bound in the CSNF matrix, which makes up the remainder of the per-package inventory. Release calculations are not valid for temperatures greater than 100C (dry conditions), with two distinct conditions for pH, pH greater than 6.8 and pH less than 6.8. With the degradation rate dependent upon: WP temperature, pH, total carbonate and oxygen fugacity.

The HLW glass waste form submodel is described in the HLW Glass Degradation Abstraction (BSC 2004 [DIRS 169988]). With the degradation rate a function of the internal inputs of WP temperature, RH, and pH.

Model Abstractions

- Dissolved Concentration Limits(6.3.7.5)

  Radionuclide solubility limits for both the waste package and invert environments are documented in *Dissolved Concentration Limits of Radioactive Elements* (SNL 2007 [DIRS 177418]). The model predicts solubility limits for 7 radioactive elements: americium, neptunium, plutonium, protactinium, radium, thorium, and uranium. For the elements carbon, cesium, iodine, strontium, actinium and technetium no solubility limits are defined (i.e. dissolved concentrations of these elements are determined by waste form release rates).

  The solubility limits for Ra, Th, Pu, Np, Am, U, and Pa are functions of environmental parameters (pH, CO2 fugacity) specific to each percolation subregion environment. Solubility limits for these species are determined within each percolation subregion environment (in addition ionic strength and [F] also affect solubility)

Model Abstractions

- EBS Colloids (6.3.7.6)

  The Waste Form and In-Drift Colloid Concentration Abstraction for the TSPA-SEIS is described in *Total System Performance Assessment Data Input Package for Waste Form and In-Drift Colloids* (SNL 2007 [DIRS 180679]) and *Waste Form and In-Drift Colloids-Associated Radionuclide Concentrations: Abstraction and Summary* (SNL 2007 [DIRS 177423]). With in the TSPA-SEIS the EBS Colloids Submodels implements abstractions to address the formation, stability and concentration of radionuclide-bearing colloids in the waste form and WP, as well as sorption of dissolved radionuclides.

  Three types of colloids:

  (1) Waste form degradation colloids:

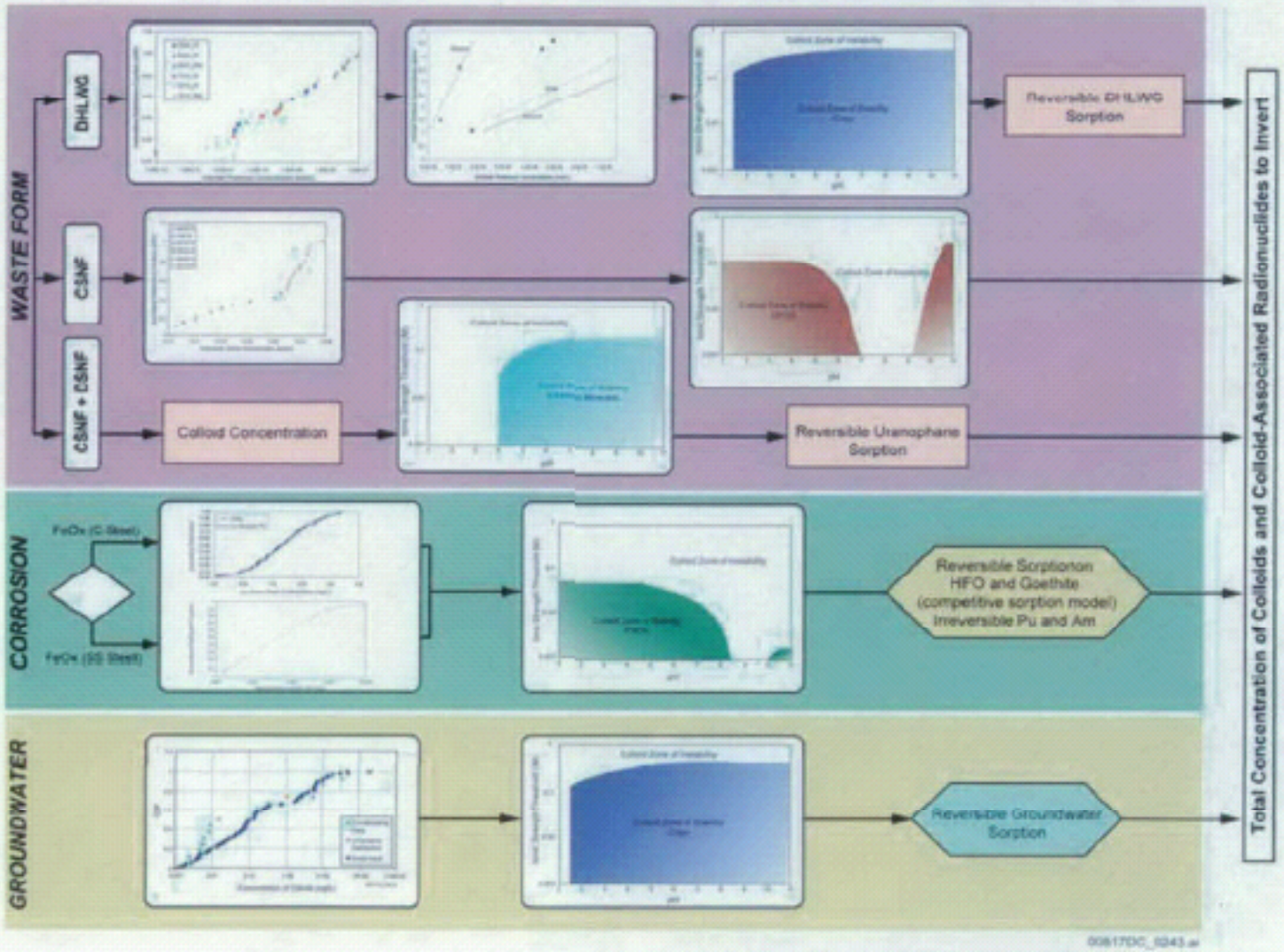
  a) Colloids generated from degradation of glass waste forms.

  b) Residue colloids generated from degradation of the CSNF waste forms.

  c) Uranium mineral colloids generated from degradation of SNF waste forms.

  (2) Colloids produced from the steel components of the WPs.

  (3) Colloids present in natural seepage water entering the EBS.



Modified from (SNL 2007 [DIRS 177423], Figure 6-17).

Figure 6.3.7-14. Logic Diagram for Computing the Concentration and Stability of All Colloids in the Waste Package

Issues relevant to colloids:

Colloid Stability – Function of ionic strength, temperature and pH

Radionuclide attachment

1) Waste form degradation colloids
    a) glass degradation colloids – reversible and irreversible
    b) CSNF degradation rind colloids – irreversible
    c) SNF uranium mineral colloids – reversible
2) Steel degradation colloids – kinetic
3) Ground water colloids – reversible

Nine elements are modeled as reversibly sorbed to colloids using linear isotherm model (Kd): Pu, Am, Cs, Pa, Th, Sn, Ra, U and Np.

The two elements most likely to impact total dose from transport of irreversibly attached colloids modeled are plutonium and americium.

Review of EBS Flow and Transport Model

The radionuclide transport through the EBS has been discretized into three primary domains.

(1) The waste form domain

CNSF-- Waste form (CSNF rods), basket tubes, absorber plates

CDSP → HLW– HLW glass, LHW glass canisters

CDSP → DSNF– DSNF, DSNF canister,

(2) The WP corrosion products domain

CNSF -- TAD canisters

CDSP – Inner vessel, support tube, outer brackets, inner brackets

(3) The invert domain

An additional domain, the EBS-UZ Interface, is included beneath the invert domain to establish a boundary condition for calculating the diffusive flux from the invert to the UZ and to compute the mass flux fraction going into the UZ fracture and matrix continua

Key Concepts and Assumptions for EBS Transport Submodel

- Radionuclide transport through each domain occurs by advection and diffusion.
- Diffusion is the primary transport mechanism when the water flux into the WP is negligibly small or zero.
- Advective transport becomes important when there is appreciable flow through the WP.
- When stress corrosion crack are the only penetrations through the DS and WP, no advective transport can occur through them.
- Advective transport can only occur when there are corrosion patch failures or when the DS and WP are damaged by igneous intrusion or ruptured by a seismic event (i.e., faulting or ground motion)
- The diffusion coefficient for the colloids is computed based on the sampled size of the colloids (SNL 2007, [DIRS 177407]).
- The amount of each radionuclide mobilized is limited by the solubility of the radionuclide in water and the amount of the RN associated with suspended colloids. Both dissolved and colloid associated radionuclide mass are transported by advection and or diffusion to the WP corrosion products domain.
- CDSP WPs have two waste form domains HLW and DSNF. These are modeled in one dimension with the HLW (glass form) feeding into the DSNF (primarily $U0_x$)

- The corrosion products domain is composed of corroded internal components of the WP, predominantly from the inner vessel and TAD canister. The internal components of a breached WP will degrade slowly over tens of thousands of years, forming corrosion products that can sorb and delay the release of RN from the WP.
- Degradation of the internal WP components results in two types of materials:
  - (1) stationary iron oxyhydroxide corrosion products that are assumed to remain in the WP
  - (2) iron oxyhydroxide colloids that are mobile and can move out of the WP
- In the invert domain RN transport occurs by both advection and diffusion and the mass flux of RN (both dissolved and colloid associated) is passed to the UZ.

Review of EBS Flow and Transport Model

The EBS Transport Submodel calculates the time-dependent mass flux of radionuclides from failed WPs through the EBS to the UZ Transport Submodel.

Inputs include:

-- Water flow through failed WPs and the underlying invert provided by the EBS Flow Submodel.

-- Temperature, RH, saturation in the invert, and imbibition flux from the host rock exiting the invert provided by the EBS TH Environment Submodel.

-- The waste form dissolution rates provided by the Waste Form Degradation Submodel.

-- Solubility limits provided by the Dissolved Concentration Limits Submodel.

-- Colloidal concentrations and sorption coefficients required to define the mobilized concentration of colloid-associated radionuclides provided by the EBS Colloids Submodel.

-- Cross-sectional area for diffusion, diffusive path lengths, porosity, water saturation, and diffusion coefficients.

Guided Tour of TSPA-SEIS

- Quick tour of TSPA Model
  - Time zero
    - Percolation subarea and seepage looping
      - EBS submodel
        - » Source calculations
        - » Degradation calculations
        - » Transport calculations

Conclusion: Identify

- Identify questions for DOE TSPA Tech exchange, and identify results and intermediate outputs necessary for an acceptance review.

- Identify areas in the model abstraction that are especially sensitive which should be given special attention during a review.