From: Keith Compton
Sent: Monday, April 24, 2006 4:16 PM
To: James Myers; David Pickett; David Brooks; Richard Codell; Tae Ahn; Christopher Grossman; Timothy McCartin
Cc: Andy Campbell; Marissa Bailey; Jack Guttmann; Bret Leslie
Subject: ENG4 Barriers Session Summary

Attached please find a bulleted summary of the ENG4 TSPA barrier analysis session. If anyone has any questions or comments please let me know...

1) Scope of ENG4
The following TSPA components are likely to be within the purview of ENG4:
- EBS Transport Abstraction
- Nuclide Inventory and Waste Package Parsing
- Cladding Degradation
- Waste Form Degradation
- In-Package Chemistry
- Colloid Generation and Stability
- EBS Solubility/In-Package & Invert
- EBS Sorption and Retardation/In-Package & Invert

The status of the EBS Flux splitting model was not clear. It belongs with either UZ2, ENG3, or ENG4; joint agreement would be needed to determine who would take ownership of it. Also, there was a brief discussion of FEPS associated with ENG4. It was suggested that association of included FEPs with these TSPA components may provide a logical way of clustering FEPs for purposes of review, rather than attempting to review each FEP individually.

2) Barrier Identification
DOE-Identified Barriers likely to be relevant to ENG4 (from EBS RTA, Table 6.7-1):
Waste Package: Limit advective and diffusive transport of radionuclides from failed waste packages by sorption onto steel internal component corrosion products
Cladding: Delay and/or limit liquid water contacting SNF after waste packages have degraded Waste Form: Limit radionuclide release rates as a result of low degradation rates for the waste forms, and low radionuclide solubilities
Invert: Limit diffusive transport of engineered barriers out of the engineered barriers by maintaining unsaturated conditions under the waste package. Limit advective and diffusive transport of radionuclides by sorption onto crushed tuff

NRC Risk Insights for ENG4
Medium: Waste form degradation rate, cladding degradation, solubility limits, and effect of colloids on waste package releases
Low: Mode of release from waste package, invert flow and transport, and criticality

3) Information to support an understanding of barrier performance General Information Recall that the EBS transport abstraction has one source term domain and three transport domains: waste form, corrosion product, and invert. The radionuclide mass can be in the following locations:

Source Term Domain
- Bound within waste form matrix in non-failed waste packages
- Bound within waste form matrix in intact cladding in packages that have failed
- Bound within waste form matrix in degraded cladding in packages that have failed

Waste Form Domain: Released into the WF domain and present as either

1) a precipitated mass;
2) a dissolved mass;
3) associated with suspended colloids; or
4) associated with destabilized colloids.

Corrosion Product Domain: Released into the corrosion product domain and present as either
1) a precipitated mass;
2) a dissolved mass;
3) associated with suspended colloids;
4) associated with destabilized colloids;
5) reversibly sorbed to corrosion products; or
6) irreversibly sorbed to corrosion products

Invert Domain: Released from the WP into the Invert and present as either
1) a precipitated mass;
2) a dissolved mass;
3) associated with suspended colloids;
4) associated with destabilized colloids;

Unsaturated Zone

Saturated Zone

Biosphere

Each of these locations is potentially associated with a barrier. A mass balance that accounted for all of these locations would yield information on where activity was retained within the system. Identifying where the mass is located in the system may provide an indication of the effectiveness of the associated barrier. Mass balances and mass fluxes are saved in the TSPA results section, and these mass balances may therefore provide an indication of the effectiveness of the different barriers for different nuclides.

Specific Information:
The following intermediate outputs may provide an indication of barrier performance associated with each component. In some cases, the outputs may be saved and the results viewed after execution. In other cases, the relevant variable can be calculated from other intermediate outputs and saved for viewing after execution. Component specific information for each of the components given above is identified below.

- EBS Transport Abstraction: mass balance (inventories and fluxes) for each of the transport compartments are saved in results section.

- Nuclide Inventory and Waste Package Parsing: Initial inventories can be examined and the distributions examined. Partitioning of inventories between bound (matrix) and unbound (gap and grain) are specified.

- Cladding Degradation: Cladding is reflected in the model as the inner barrier in the source term element. The fraction of inner barrier failed is an intermediate output.

- Waste Form Degradation: Time histories of degradation rates can be saved; the fraction of waste degraded is computed and can be examined.

- Colloid Generation and Stability: Ionic strength and pH can be examined to identify whether colloid stabilitiy limits would have ever been exceeded. We should be able to track total colloid mass over time. However, it is not clear how to identify the colloid associated radionuclide mass. Relation of colloidal transport to any particular barrier is not yet clear; would need to think about how to apply barrier analysis to an evaluation of colloidal transport.

- EBS Solubility/In-Package & Invert: Solublities are defined with respect to the transport fluid. Time histories of EBS and invert solubility and the time-dependent amount of precipitated mass in each transport cell can be saved.

- EBS Sorption and Retardation/In-Package & Invert: Distribution coefficients are defined in the Materials container. Sorption can occur to smectite colloids (GW and waste glass colloids), reversibly and irreversibly to stationary and colloidal corrosion products, and reversibly to porous media materials. Time histories of distribution coefficients can be saved. It is not clear now to extract the amount of mass reversibly or irreversibly sorbed within a transport pathway. Would need integration with UZ3 to evaluate invert sorption, since invert distribution coefficients are based on the values sampled for the UZ transport component.

- In-Package Chemistry: time histories of pH and ionic strength can be saved. In package chemistry does not represent a barrier in and of itself; however, it determines the performance of other barriers (e.g., solubility, colloidal stability, waste form degradation, etc.). Since the impact of in-package chemistry on different barriers can be highly non-linear (e.g., colloidal stability exhibits a pH-dependent ionic strength threshold), the impact of using a single "representative" chemistry to represent the heterogeneity of chemical conditions across an ensemble of waste packages is a potential subject for further examination.

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