

Scientific Analysis
Administrative Change Notice

Complete only applicable items.

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1. Document Number:	ANL-WIS-MD-000009	2. Revision:	02	3. ACN:	01
4. Title:	Waste Form Features, Events, and Processes				
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6. Approvals:

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7. Affected Pages	8. Description of Change:
6-34	<p>Corrected typographical error (No DIRS impact) The DIRS citation in Section 6.2.17 (under "Screening Argument," first bullet, last sentence) is incorrectly identified as:</p> <p>"Additionally DSNF will be widely dispersed throughout the repository, as will any produced flammable gas (BSC 2004 [DIRS 170020], Section 6.2.17)."</p> <p>This is a typographical error. The correct DIRS citation is:</p> <p>Additionally DSNF will be widely dispersed throughout the repository, as will any produced flammable gas (BSC 2004 [DIRS 170022], Section 6.2.17).</p> <p>This error was identified in CR 4236.</p>
4-3	<p>Incorrect citation (correct DIRS as appropriate) Table 4-1, for DIRS entry 169425, under "used from" column, 4th cell, change:</p> <p>Sections 6.3.2 and 6.6.4.5 To Sections 6.3.2 and 6.6.5.4</p> <p>This correction is associated with TBV-6293.</p>
6-44	<p>Incorrect citation (correct DIRS as appropriate) 2nd paragraph, 2nd sentence, change:</p> <p>(BSC 2004 [DIRS 169425], Section 6.6.4.5) To (BSC 2004 [DIRS 169425], Section 6.6.5.4)</p> <p>This correction is associated with TBV-6293.</p>

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4. Title:	Waste Form Features, Events, and Processes				
4-4	<p>Incorrect citation (correct DIRs as appropriate) Table 4-1, for DIRS entry 167621, under "used from" column, 8th cell, change:</p> <p><i>Sections 4.1.2, 6.6.2 and Table 10</i> To: <i>Section 6.6.4</i></p> <p>This correction is associated with TBV-6295.</p>				
6-59	<p>Incorrect citation (correct DIRs as appropriate) Section 6.2.39, under "Supporting Documents" header, change:</p> <p><i>"In-Package Chemistry Abstraction (BSC 2004 [DIRS 167621]). While FEP 2.2.08.12.0B is not in the included FEP table (BSC 2004 [DIRS 167621], Table 10), it is addressed in the report."</i></p> <p>To</p> <p><i>"In-Package Chemistry Abstraction (BSC 2004 [DIRS 167621]). While FEP 2.2.08.12.0B is not in the included FEP table (BSC 2004 [DIRS 167621], Table 6-1), it is addressed in the report."</i></p> <p>This correction is associated with TBV-6295.</p>				

Table 4-1. Direct Inputs (Continued)

Technical Product Input	Used From	Used In	Input Description	
BSC 2004 [DIRS 169425]	Section 6.5.3.2	Section 6.2.22	Use of adjusted Eh model to account for redox potential in the repository	
	Section 6.3.2	Section 6.2.23	Consideration of kinetics in the solubility model	
	Sections 6.3.2, 6.5 through 6.18	Table 4-1, Section 6.2.21	Abstraction of solubility models for 14 elements (plutonium, neptunium, uranium, thorium, americium, actinium, protactinium, radium, technetium, iodine, strontium, carbon, and cesium) may be used to constrain the maximum radionuclide concentrations.	
	Sections 6.3.2 and 6.5.4	Table 4-1, Sections 5.2, 6.2.24	Alternative model (not utilized in the base-case) of incorporation of neptunium into uranyl minerals that captures the experimental results very well, and eliminates the built-in conservatism in the conventional pure phase solubility approach and thus gives more realistic source terms.	
	Section 6.4	Table 4-1, Section 6.2.35	Parameterizes dissolved concentrations of radionuclides as a function of in-package and EBS solution chemistry over a range of carbon dioxide partial pressures of 10^{-5} to $10^{-1.5}$ - in effect to two orders of magnitude greater than atmospheric.	
	Section 6.4	Table 4-1, Section 6.2.39	The dissolved concentration model considers the potential chemistry of water entering the waste package.	
	Table 6.4-5	Section 6.2.38, Table 4-1	Neutron flux at the waste package surface	
	Section 8.1	Section 6.2.5	Naval fuel is conservatively treated as CSNF	
	Section 8.1	Sections 6.2.5 and 6.2.32	DSNF is released in a single TSPA-LA timestep	
	Table 6-2	Sections 6.2.8 and Table 4-1	Uranium metal corrosion rate	
BSC 2004 [DIRS 169593]	Section 6.1.12	Section 6.2.3	DSNF is released within one TSPA-LA time step, so is not sensitive to surface area	
	Section 6.1	Section 6.2.5, Table 4-1	Development of upper-limit and best estimate degradation models for each of 11 DSNF Waste Groups for TSPA-LA.	
	Section 6.2	Sections 6.2.16, 6.2.18, Table 4-1	Rapid corrosion rate of the metallic uranium that is the matrix of N Reactor DSNF compared with other SNF.	
	Section 6.4.3	Section 6.2.15, Table 4-1, and Appendix B	Lack of sufficient available information to adequately characterize N Reactor spent fuel cladding.	
	Section 8.1	Section 6.2.3, Table 4-1	The DSNF release rate model has no explicit dependence on water chemistry effects that could result from chemical interactions between or within waste packages.	
	BSC 2004 [DIRS 167618]	Section 8.1	Section 6.2.3, Table 4-1	The DSNF release rate model has no explicit dependence on water chemistry effects that could result from chemical interactions between or within waste packages.

Table 4-1. Direct Inputs (Continued)

Technical Product Input	Used From	Used In	Input Description
BSC 2004 [DIRS 167621]	Sections 4.1 and 6.6.2	Section 6.2.39	Various water compositions entering the waste package
	Sections 6.3.1.1, 6.6.4, 6.10.2.3	Section 6.2.22	Discussion of redox potential in the in-package chemistry mode
	Sections 4.1.3, 4.1.4, 6.6, 6.3.1.1, 6.6.3, and 6.10.2.3	Section 6.2.23	Discussion of kinetics in the in-package chemistry model
	6.4.1	Section 6.2.34	Convection on the in-package chemistry model
	Sections 6.3.1, 6.6.1, and 6.6.4	Section 6.2.13	Discussion of modeling voids in the waste package
	Appendix B	Section 6.2.37	Radiolysis analysis show negligible impact on In-Package chemistry
	Section 6.5	Table 4-1 and Section 6.2.3	Support for the conclusion that HLWG tends to generate high pH solutions while DOE SNF generates neutral pH solutions, and together combined with the waste package materials the high pH values are buffered to lower values. Also, the DSNF codisposal and high-level radioactive waste glass waste packages are expected to be generally cooler than commercial SNF packages at the time of disposal
	Section 6.6.4	Table 4-1, Section 6.2.35	Support for the conclusion that it is reasonable to expect little impact of carbon dioxide production on in-package pH and ionic strength, and that only minor amounts of organic materials might appear in the WP.
	Section 6.10 and 6.3.1	Table 4-1, Section 6.2.33	Temperature effect on the in-package model
	Entire	Table 4-1, Sections 6.2.3, 6.2.13, and 6.2.19	General reference describing the basis of the conceptual model for in-package chemistry of water.
	Section 6.7 and 7, Table 6-2, Appendices I.4.2 and I.5, Table 7-1	Sections 6.2.1, 6.2.2, 6.2.3, 6.2.4, 6.2.8, 6.2.16, 6.2.17, 6.2.40 and Table 4-1	Provides the inventories of radionuclides for three major categories of waste forms, currently planned for disposal at Yucca Mountain: CSNF, DSNF, and DHLW Glass.
	Appendix I (I.4 and I.5)	Section 6.2.1	Crud deposits not significant
	Table 6-3	Section 6.2.3	Some WPs will contain 5-HLWG and no DSNF
Table 6-1	Section 6.2.40	Radionuclide precursors	

percent of the total waste; therefore, waste stream plume chemistry is dominated by the CSNF waste even when bounding DSNF degradation models are used.

Supporting Documents:

DSNF and Other Waste Form Degradation Abstraction (BSC 2003 [DIRS 167618])

Initial Radionuclide Inventories (BSC 2004 [DIRS 170022])

6.2.17 Flammable Gas Generation from DSNF (2.1.02.29.0A)

FEP Description:

DSNF to be disposed in Yucca Mountain will contain a small percentage of carbide fuel. When carbide is exposed to water, flammable gases such as methane and its minor constituents ethane, ethylene, and acetylene (referred as ethyne by the International Union of Pure and Applied Chemistry) are generated. If these gases ignite, localized increases in temperature can occur, which might affect fuel degradation. The area around the ignition point may be mechanically and/or thermally perturbed, which could affect waste package or host-rock properties in the adjacent area of the EBS.

Screening Decision:

Excluded (low consequence)

Screening Argument: Flammable-gas generation based on the reaction of DSNF carbide fuel with liquid water or water vapor can be excluded based on low consequence for the following reasons:

1. The only fuel waste types capable of producing organic flammable gasses such as methane, ethane, etc., are the uranium-thorium carbide and the plutonium-uranium carbide DOE SNF waste fuels because they are the only spent nuclear fuels containing more than trace quantities of carbon. These gasses are formed by the reaction of the carbides with liquid water or water vapor. Only a small percentage (approximately 1 percent or 25 MTHM) of DSNF fuel contains U/Th carbide fuels and there is only about 100 kg of Pu/U carbide DSNF (DOE 2002 [DIRS 158405], Table D-1). The carbide spent nuclear fuels will be present in about 5 percent of the waste packages (DOE 2004 [DIRS 169354], p. D-580). Additionally DSNF will be widely dispersed throughout the repository, as will any produced flammable gas (BSC 2004 [DIRS 170022], Section 6.2.17).
2. Additionally, the repository is located in fractured and unsaturated tuffaceous rock (DOE 2002 [DIRS 155943], Section 1.4.2.2.2). This rock is overlaid by approximately 250 meters of unsaturated welded and nonwelded tuffs. With the exception of intermittent perched zones, both the matrix and the fractures within the host rock above and below the repository horizon have a relatively high degree of gas saturation (generally greater than 50 percent), making these areas more gas permeable than liquid permeable. Within the repository horizon, ambient gas saturation in the matrix ranges between 10 to 20 percent, while gas saturation in fractures tends to be much higher. These conditions will promote a dispersive gas flow path between the

Finally, Chen (2001 [DIRS 161997]) and Chen et al. (2002 [DIRS 161996]) analyzed the relative release rates of neptunium and uranium in the fuel degradation experiments referred to above and found a close correlation between neptunium and uranium concentrations in the leachates. In other words, the ratio of neptunium to uranium in the leachate is equal to the ratio in the spent nuclear fuel used in the experiments. Bruno et al. (1998 [DIRS 101565]) have also observed a coherent relation between neptunium and uranium in spent nuclear fuel dissolution experiments in the Spanish Nuclear Waste Program. These results are corroborated by the linear relationship between neptunium contents in uranophane and Na-compreignacite and the mother solution that was found by Buck et al. (2003 [DIRS 168411]).

An alternative model of accounting for incorporation of neptunium into uranyl minerals was generated based on experimental data. The results produced by the alternative model capture experimental results well (BSC 2004 [DIRS 169425], Section 6.6.5.4). It eliminates the built-in conservatism in the conventional pure phase solubility approach and, thus, gives more realistic source terms. However, experimental studies on whether schoepite, the critical secondary uranyl phase, can incorporate and immobilize sufficient neptunium during spent nuclear fuel corrosion do not provide a solid basis for recommending this model to be used in the TSPA-LA model. Experimental work leading to data bearing on this model is under continuous review and may lead to an amended recommendation to adopt neptunium concentrations based on the coprecipitation model.

In summary, although the inclusion of secondary-mineral phases in the TSPA-LA would reduce calculated doses because these solids have the ability to sequester radionuclides, no credit is taken for this process in the TSPA-LA. Therefore, secondary-phase effects on dissolved radionuclide concentrations are excluded from the TSPA-LA based on low consequence because they have no adverse effects on performance.

TSPA Disposition:

N/A

Supporting Documents:

N/A

6.2.25 Complexation in EBS (2.1.09.13.0A)

FEP Description:

The presence of organic complexants in water in the EBS could augment radionuclide transport by providing a transport mechanism in addition to simple diffusion and advection of dissolved material. Organic complexants may include materials found in natural groundwater such as humates and fulvates, or materials introduced with the waste or engineered materials.

Screening Decision:

Excluded (low consequence)

Screening Argument: Repository temperatures are expected to remain sufficiently high that significant microbial activity is possible only after the first 1,000 years, when the drift temperature drops below the approximate 96°C boiling point (BSC 2004 [DIRS 169991],

TSPA Disposition:

Six different initial water compositions were used to represent the chemistry of the water flowing into the waste package. The base case considers three water compositions, and a sensitivity study (BSC 2004 [DIRS 167621], Section 6.6.2) considers an additional three water compositions. This inflowing water chemistry is one of the inputs used to determine the in-package chemistry in the IPCM. Therefore, the variability of the incoming water composition is implicitly included in the in-package chemistry and in the abstractions passed to TSPA-LA in *In-Package Chemistry Abstraction* (BSC 2004 [DIRS 167621]). TSPA-LA then feeds these results to the solubility, colloid, CSNF, and HLW glass submodels. The effects of the inflowing water chemistry are captured within the IPCM parameters: pH, ionic strength, total carbonate, Eh, chloride, and fluoride.

The water influx model examined various input water chemistries (BSC 2004 [DIRS 167621], Section 4.1.2) and their effect on the in-package chemistry. The results showed the parameters passed to TSPA-LA were unaffected by changes in the input water composition. Thus, while the composition of the water flowing into the waste package is implicitly included in the TSPA-LA model, variations in the composition do not significantly affect the model results.

The dissolved concentration report considers the chemistry of the water potentially entering a waste package (BSC 2004 [DIRS 169425], Section 6.4). Various sensitivities were performed to examine the effect of compositions of 25 pore water compositions (Section 6.4.2.5). For the species that have an impact on solubility, an uncertainty term was developed (Sections 6.4.3.6 and 6.4.6.7) to account for the variation of that species in the incoming water.

Supporting Documents:

In-Package Chemistry Abstraction (BSC 2004 [DIRS 167621]). While FEP 2.2.08.12.0B is not in the included FEP table (BSC 2004 [DIRS 167621], Table 6-1), it is addressed in the report.

Dissolved Concentration Limits of Radioactive Elements (BSC 2004 [DIRS 169425])

6.2.40 Radioactive Decay and Ingrowth (3.1.01.01.0A)

FEP Description:

Radioactivity is the spontaneous disintegration of an unstable atomic nucleus that results in the emission of subatomic particles. Radioactive isotopes are known as radionuclides. Radioactive decay of the fuel in the repository changes the radionuclide content in the fuel with time and generates heat. Radionuclide quantities in the system at any time are the result of the radioactive decay and the growth of daughter products as a consequence of that decay (i.e., ingrowth). Over a 10,000-year performance period, these processes will produce daughter products that need to be considered in order to adequately evaluate the release and transport of radionuclides to the accessible environment.

Screening Decision:

Included

Screening Argument:

N/A