OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
ANALYSIS/MODEL COVER SHEET
Complete Only Applicable Items

1. QA: QA
Page: 1 of: 10

2. ☒ Analysis — Check all that apply		3. ☒ Model — Check all that apply	
Type of Analysis	☐ Engineering ☒ Performance Assessment ☐ Scientific	Type of Model	☒ Conceptual Model ☐ Abstraction Model ☐ Mathematical Model ☐ System Model ☐ Process Model
Intended Use of Analysis	☐ Input to Calculation ☒ Input to another Analysis or Model ☐ Input to Technical Document ☐ Input to other Technical Products	Intended Use of Model	☐ Input to Calculation ☒ Input to another Model or Analysis ☐ Input to Technical Document ☐ Input to other Technical Products
Describe use: Description of implementation of water volume in rind pore spaces of wasteform to be implemented in total systems performance model for SR.		Describe use: Description of implementation of water volume in rind pore spaces of wasteform to be implemented in total systems performance model for SR.	

4. Title:
In-Package Source Term Abstraction

5. Document Identifier (including Rev. No. and Change No., if applicable):
ANL-WIS-MD-000018 Rev 00

6. Total Attachments:	7. Attachment Numbers - No. of Pages in Each:
None	N/A

	Printed Name	Signature	Date
8. Originator	Rick Reeves	Signature	Date 6/8/00
9. Checker	Haywood Anderson	for	6/8/00
10. Lead/Supervisor	Robert Rechard		6/9/00
11. Responsible Manager	Bob MacKinnon		6/20/00

12. Remarks:
Rev 00

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
ANALYSIS/MODEL REVISION RECORD

Complete Only Applicable Items

2. Analysis or Model Title: In-Package Source Term Abstraction

3. Document Identifier (including Rev. No. and Change No., if applicable): ANL-WIS-MD-000018 REV 00

4. Revision/Change No.	5. Description of Revision/Change
Rev 00A	Check Copy
Rev 00B	Back Check Copy and Review Copy
Rev 00C	Final Check Copy and Concurrence Copy
Rev 00	Initial Issue

CONTENTS

Page

1. PURPOSE 4

2. QUALITY ASSURANCE 4

3. COMPUTER SOFTWARE AND MODEL USAGE 4
   - 3.1 COMPUTER SOFTWARE 4
   - 3.2 MODELS 4

4. INPUTS 5
   - 4.1 DATA AND PARAMETERS 5
   - 4.2 CRITERIA 5
   - 4.3 CODES AND STANDARDS 5

5. ASSUMPTIONS 6

6. ANALYSIS/MODEL 6
   - 6.1 PREVIOUS WORK 6
   - 6.2 NEW CONCEPTUAL MODEL 7
   - 6.3 WASTEFORM POROSITY 8
   - 6.4 CONCEPTUAL MODEL VALIDATION 8

7. CONCLUSIONS 9

8. REFERENCES 9

1. PURPOSE

The purpose of this conceptual model analysis is to assist Performance Assessment Operations (PA) in modeling the volume of in-package water available for contact with the wasteform. The conceptual model developed in this analysis model report (AMR) represents an enhancement of the in-package water volume model that was abstracted into TSPA-VA performance assessment modeling. This enhanced conceptual model will allow PA to provide a more detailed and complete representation of the volume of in-package water available for contact with the wasteform as a function of time. The conceptual model is presented as a methodology appropriate for use in the total system performance model.

This analysis was conducted in response to the written work direction in the *Technical Development Plan, In-Package Source Term Abstraction, TDP-WIS-MD-000029* (CRWMS M&O 1999a).

2. QUALITY ASSURANCE

This Performance Assessment (PA) activity has been evaluated to the requirements of QAP-2-0 *Conduct of Activities* (QAP-2-0, Rev. 5) and is subject to *Quality Assurance Requirements and Description* (DOE 2000) requirements. The documentation of this analysis is in accordance with the guidance given in AP 3.1Q *Conduct of Performance Assessment* (AP 3.1Q Rev 0, ICN 1) and the directions found in AP 3.10Q *Analyses and Models* (AP 3.10Q Rev 2) and thus implements the requirements given in the QARD for analysis activities.

3. COMPUTER SOFTWARE AND MODEL USAGE

3.1 COMPUTER SOFTWARE

No computer software was used in developing this enhanced conceptual model.

3.2 MODELS

The conceptual model discussed in this analysis represents an enhancement of the in-package water volume methodology used in the TSPA-VA Base Case Model. The new methodology developed here accounts for different waste package failure times. Also, this methodology can be used to incorporate the rate of cladding failure for commercial spent fuel (CSNF) when determining rind water volume for CSNF. This enhanced methodology will be implemented in the total system performance model in TSPA-SR.

The previous methodology used for determining the volume of in-package water available for contact with the wasteform in performance assessment modeling for TSPA-VA is documented in *Total System Performance Assessment – Viability Assessment Base Case* (CRWMS M&O 1998a). The methodology discussed in the aforementioned document is being replaced by the methodology developed in this AMR; as such, the model discussed in the TSPA-VA Base Case document is used here only as a reference point from which to extract a discussion of the previous treatment used to determine the volume of in-package water available for contact with the wasteform in the base case. The only changes between the model presented here and the TSPA-VA Base Case model concern the methodology used to account for different package failure times (and, in the case of CSNF, rate of cladding failure) in determining the rind volume of the wasteform within the total system performance model used to assess Engineered Barrier System (EBS) performance.

4. INPUTS

4.1 DATA AND PARAMETERS

There are no data nor parameter values used in the development of this conceptual model. Parameter names used for the purpose of describing the methodology are presented in Section 6 of this report, and represent the same parameter names used in *Total System Performance Assessment – Viability Assessment Base Case* (CRWMS M&O 1998a).

4.2 CRITERIA

This AMR was prepared to comply with the DOE Interim Guidance (Dyer 1999) which requires the use of specified subparts/sections of the proposed NRC High-Level Waste Rule 10 CFR 63 (64 FR 8640). Subparts of this proposed rule that are particularly applicable to models/analyses are outlined in Subpart E, Sections 114 (Requirements for Performance Assessment) and 115 (Characteristics of the Reference Biosphere and Critical Group), of the Interim Guidance Document.

4.3 CODES AND STANDARDS

There are no codes nor standards referenced in this report.

5. ASSUMPTIONS

The following assumptions are used in the development of the conceptual model presented in this analysis, and are used throughout the analysis.

1) The abstracted methodology for determining the volume of in-package water available for contact with the wasteform is based on the same assumptions and approximations shown appropriate for TSPA-VA.

2) The volume of in-package water available for contact with the wasteform, as represented in total systems modeling by the water in the wasteform mixing cell for a particular inventory type for a particular repository region, is assumed to be equal to the pore space of the rind of alteration products forming on the wasteform. The volume of in-package water available for contact with the wasteform is therefore the rind volume times the porosity times the water saturation. This assumption is based on the fact that any rind forming on the wasteform will not be a layer composed solely of in-package water, but rather will be a rind of altered fuel wherein water has penetrated via pore spaces.

3) Wasteform mass is evenly distributed throughout the wasteform. This assumption is necessary for calculating rind volume given the method in which RIP internally performs wasteform calculations using fraction of mass at a given time step.

4) While this AMR describes a conceptual model and does not consider actual parameter values, a possible value for porosity of the wasteform is 20%. The actual value of porosity has no impact on the conceptual model, and is given here due to the fact that a value for porosity has not been captured in any other AMR. The basis for this 20% porosity value can be found in DTN: LL000207751021.119 .

6. ANALYSIS/MODEL

6.1 PREVIOUS WORK

As described in the TSPA-VA Technical Basis Document, *Chapter 6: Wasteform Degradation, Radionuclide Mobilization, and Transport through the Engineered Barrier System* (CRWMS M&O 1998b), the TSPA-VA Base Case Model uses a single mixing cell to represent the wasteform for a group of waste packages for each wasteform inventory type for each region of the repository (i.e., there are three inventory types in each of six regions, with a mixing cell for each inventory type representing the wasteform). This mixing cell is scaled in size to the number of waste packages that have breached within that inventory type. As more waste packages breach, the size of the mixing cell increases to account for the volume and inventory of the newly breached waste package. Cells within the total system model are defined with a volume of water and mass of solid materials associated with the cell. The amount of water in the wasteform mixing cell (i.e., the volume of in-package water available for contact with the wasteform) is assumed to be equal to the pore space of the rind of alteration products that forms as the UO_2 is converted into secondary minerals. The volume of in-package water available for contact with

the wasteform at any given time following package breach is represented by this rind water volume, which grows over time as the wasteform dissolves. The volume of water in the rind is used in the calculation of dissolved mass concentrations for mass degraded from the wasteform. These calculated concentrations are compared to the solubility limited concentrations of radionuclides of interest from the degraded wasteform for determination of aqueous release concentrations to the engineered barrier system outside the waste package.

The methodology for calculating the rind volume in the TSPA-VA Base Case Model is described in the *Total System Performance Assessment – Viability Assessment Base Case* (CRWMS M&O 1998a). In the TSPA-VA model, mass of wasteform exposed (degraded) at each time step is calculated in the Integrated Probabilistic Simulator for Environmental Systems, also known as RIP (CRWMS M&O 1999b), using the product of three parameters: fuel degradation rate, fuel rod mass, and time since time zero. RIP calculates the fraction of exposed wasteform at each time step using the degradation rate (which is in units of fraction of mass degraded per year). Since it is assumed that mass is evenly distributed throughout the wasteform, the fraction of wasteform mass degraded equals the fraction of wasteform volume degraded. This fraction of wasteform volume degraded represents the rind of alteration products. Thus, in the TSPA-VA model, rind volume is the product of fuel degradation rate, fuel rod volume, and time since time zero (absolute time).

Rind volume = [fuel degradation rate, fraction/yr]*[fuel rod volume, m^3 (a constant)]*[time since time zero, yr]

The volume of water in the rind is the rind volume times porosity times the water saturation.

6.2 NEW CONCEPTUAL MODEL

The conceptual model for calculating volume of in-package water available for contact with the wasteform to be used for TSPA-SR is an enhanced version of that used for TSPA-VA. The enhancement has to do with a more appropriate method of accounting for packages coming on-line (i.e., available for degradation once the wasteform is exposed due to waste package failure or, in the case of CSNF, cladding failure) at different points in time for use in the total system performance model. The methodology as defined in terms of parameters remains unchanged. Rind volume is still calculated using fuel degradation rate, fuel rod volume, and time.

The difference in TSPA-SR implementation is that the time term is no longer *absolute time or time since time zero*; instead, time is *the length of time since the wasteform became available for degradation.* This represents a more appropriate method for calculating rind volume in terms of waste packages coming on-line, and results in the wasteform mass from the different waste packages undergoing degradation at different points in time since time zero.

For each waste package, the rind volume at any point in time is a function of the wasteform degradation rate and the time of exposure. Thus, any enhancement of the TSPA-VA conceptual model should account for rind volumes coming on-line at different points in time as wasteform is exposed due to package failure or – in the case of CSNF – cladding failure rate. Since rind volume is a function of exposed mass, the conceptual model for rind volume for each waste package is the fraction of exposed mass over total mass multiplied by the rod volume.

Multiplication of the exposed mass fraction by wasteform porosity and water saturation gives the volume of water in the rind available for contact with the wasteform:

Water volume in the wasteform rind = [exposed mass fraction]*rod volume*porosity*water saturation

Note that time is accounted for in the exposed mass fraction term.

If, in TSPA-SR, the total system performance model is implemented in terms of unexposed mass for each wasteform in a waste package at each time step, the methodology must be implemented in terms of exposed mass by subtracting the fraction of unexposed mass from 1:

Water volume in the wasteform rind = [1 – (unexposed mass fraction)]*rod volume*porosity*water saturation

for all waste packages of each wasteform inventory type in each repository region.

Note that, for CSNF, this methodology (whether in terms of exposed or unexposed wasteform mass fraction) accounts for rate of cladding failure by allowing the total system model to determine the mass fraction at each time step for each waste package depending on the cladding failure rate.

6.3 Wasteform Porosity

Actual parameter values are irrelevant to the methodology presented here. However, because it has not been recorded in any other AMR, a suggested value for porosity of 20% is presented as part of this AMR. The basis for this 20% porosity value can be found in DTN: LL000207751021.119.

6.4 Conceptual Model Validation

In the CSNF Cladding Degradation Component, the HLW Degradation Component, and the DSNF Degradation Component of the Waste Form Degradation Model for the TSPA-SR analysis, the mass of radioisotope liberated from CSNF, HLW, and DSNF is evaluated. The TSPA-SR performance assessment model must convert this liberated mass of a radioisotope into a concentration. For the purposes of the TSPA-SR performance assessment model, the mixing cell volume for evaluating the concentration is the volume of void space in the altered (or "rind") of the CSNF, HLW, and DSNF rather than the entire void space that may be present in a waste package. For the CSNF, this volume would be the portion of the SNF rod that had been exposed through cladding unzipping and alteration from UO_2 to schoepite. That is, only the volume of water in direct contact with CSNF, HLW, or DSNF is assumed to determine the concentration of the dissolved radioisotope (Assumption 2, above). This assumption conservatively assumes a very small volume for the mixing cell, and, thereby, ensures a conservatively high concentration that is at or very near the solubility limit of the radioisotope. In the performance assessment

model, this concentrated packet of water leaves the waste package without further dilution at the rate water enters the package. Because the conceptual model is conservative, it is adequate for the intended purpose of supporting the site recommendation of Yucca Mountain.

7. CONCLUSIONS

The methodology presented here for calculating the volume of in-package water available for contact with the wasteform is an enhanced version of that used in the TSPA-VA Base Case Model. In the TSPA-VA Base Case Model, as implemented using the RIP code, rind volume is calculated using the product of fuel degradation rate, fuel rod volume, and time since time zero. This value of rind volume is calculated independently for each time step.

In the analysis presented here, the implementation is enhanced such that the time term in the rind calculation is no longer *time since time zero (or absolute time)*; instead, the time term is *the length of the time since the wasteform became available for degradation.* This represents a more appropriate method for calculating rind volume in terms of how waste packages fail at different times over the life of the repository. This methodology also accounts for rate of cladding failure for CSNF packages for determining exposed mass. The volume of water in the rind for each wasteform type in a waste package at any time step is a function of the fraction of exposed wasteform multiplied by the volume of rods, the porosity, and the water saturation of the wasteform.

Although the conceptual model presented here does not depend on values for individual parameters, one possible value for wasteform porosity is 20% (Assumption 4).

Note: AP-3.15Q requires the following statement be added to all products containing unresolved TBVs (To Be Verified):

"This document may be affected by technical product input information that requires confirmation. Any changes to the document that may occur as a result of completing the confirmation activities will be reflected in subsequent revisions. The status of the input information quality may be confirmed by review of the Document Input Reference System Database."

This statement is required by procedure; however, whether or not the 20% porosity value is confirmed as verified does not impact the conceptual model.

8. REFERENCES

64 FR (Federal Register) 8640. Disposal of High-Level Radioactive Wastes in a Proposed Geologic Repository at Yucca Mountain, Nevada. Proposed rule 10 CFR 63. Readily Available.

AP 3.1Q, Rev. 0, ICN 1. *Conduct of Performance Assessment.* Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.19990304.0214.

AP-3.10Q, Rev. 2. *Analyses and Models.* Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.19991028.0012.

AP-3.15Q, Rev. 1. *Managing Technical Product Inputs* . Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20000218.0069.

CRWMS M&O 1998a. *"Total System Performance Assessment – Viability Assessment Base Case"* B00000000-01717-0210-00011 Rev 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19981202.0279.

CRWMS M&O 1998b. *"Waste Form Degradation, Radionuclide Mobilization, and Transport Through the Engineered Barrier System."* Chapter 6 of *Total System Performance Assessment – Viability Assessment (TSPA-VA) Analyses Technical Basis Document* B00000000-01717-4301-00006 Rev 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19981008.0006.

CRWMS M&O 1999a. *In-Package Source Term Abstraction*, TDP-WIS-MD-000029 Rev 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19991008.0219.

CRWMS M&O 1999b. *Software Qualification Report for Repository Integration Program (RIP)*, Version 5.19.01 CSCI: 30055V5.19.01 ACC: MOL.19980916.0337.

DOE (Department of Energy) 2000. *Quality Assurance Requirements and Description.* DOE/RW/0333P. Rev. 10. Washington, D.C.: U.S. Department of Energy. ACC: MOL.20000427.0422.

Dyer, J.R. 1999. "Revised Interim Guidance Pending Issuance of New U.S. Nuclear Regulatory Commission (NRC) Regulations (Revision 01, July 22, 1999) for Yucca Mountain, Nevada." Letter from J. Russell Dyer (DOE) to D.R. Wilkins (YMP), September 3, 1999, OL&RC:SB-1714, with enclosure, "Interim Guidance Pending Issuance of New NRC Regulations for Yucca Mountain (Revision 1)." ACC: MOL.19990910.0079.

QAP-2-0, Rev. 5. *Conduct of Activities.* Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.19980826.0209.

DTN: LL000207751021.119. CSNF Alteration Phase Porosity Estimate. Scientific Notebook LLNL-SCI-433. Select pages submitted as a data package with accompanying explanation.