EVALUATION OF GOLDSIM IMPLEMENTATION OF TOTAL SYSTEM PERFORMANCE ASSESSMENT–SITE RECOMMENDATION—CNWRA INPUT

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ABSTRACT

This report reviews the consistency between the U.S. Department of Energy (DOE) TSPA–GoldSim code and the supporting documentation for particular submodels of the code. This review activity is part of a joint effort by the U.S. Nuclear Regulatory Commission (NRC) and Center for Nuclear Waste Regulatory Analyses (CNWRA) staffs. This report summarizes only review activities by the CNWRA staff. These review activities are consistent with review methods in the draft Yucca Mountain Review Plan (NRC, 2002a) concerning the demonstration of compliance with the postclosure individual protection standard. The review activities included inspection of an electronic file containing a single-realization run of the DOE TSPA–GoldSim code, with stochastic variables fixed at their median values. The review was split into two areas, model input and model implementation, consistent with a review outline developed by the NRC staff. For model input verification, a selected sample of data and expressions of the DOE TSPA–GoldSim code was traced to documentation sources. Similarly, the model implementation activity checked the submodel function and representation with respect to the DOE documentation of the TSPA–GoldSim code. The submodels reviewed included (i) the radionuclide inventory abstraction, (ii) igneous activity, (iii) waste package and drip shield degradation, (iv) colloid release and transport in the engineered barrier subsystem, and (v) the biosphere model. Submodels (i) and (ii) were reviewed for model input only. Model implementation review activities for submodels (iii), (iv), and (v) included constructing a simplified model to emulate the implementation of the general corrosion model; comparing colloid model verification results in the site recommendation document to outcomes predicted by process model abstraction reports; tracing information flow from the saturated zone model to the biosphere model; and verifying with hand calculations groundwater concentration, water usage, and dose estimates in the biosphere model. No inconsistencies were found in (ii). Inconsistencies between the DOE documentation and the TSPA–GoldSim implementation found in submodels (i), (iii), and (iv) related to lack of documentation or disagreement of parameter values and distributions and lack of correspondence in the model description. In (v), disagreement with the final release of 10 CFR Part 63 (NRC, 2001) was noted; however, DOE is planning to incorporate final regulations into the TSPA–GoldSim code.

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QUALITY OF DATA: Sources of data are referenced in each chapter. Data from non-CNWRA sources are freely used. The respective sources of non-CNWRA data should be consulted for determining levels of quality assurance.

ANALYSES AND CODES: Mathematica® Version 4.1 (Wolfram Research, Inc., 1999) and Microsoft® Excel® 97 were used for analyses contained in this report. Mathematica® Version 4.1 is a commercial software for general mathematical analyses. Excel® 97 was used to perform simple arithmetic computations and create plots. Mathematica® and Excel® 97 are general-use software and are not under TOP–18 control. Procedures developed in Mathematica® Version 4.1 were constructed to perform statistical analyses and calculations associated with a simplified model to simulate general corrosion. Details concerning these procedures can be found in CNWRA scientific notebook number 493. GoldSim Version 1.30.1 (GoldSim Technology Group, 2002) was used for this review.

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EXECUTIVE SUMMARY

This report is review of consistency of the U.S. Department of Energy (DOE) documentation and the total system performance assessment code implemented in the GoldSim platform (code referred to as TSPA–GoldSim code in this report). To that aim, an electronic file (SR00_037ne6.gsm) containing results from a single realization run of the TSPA–GoldSim code, with input parameters fixed at their median values, and supporting documentation were inspected. This review activity is part of a joint effort by the U.S. Nuclear Regulatory Commission and Center for Nuclear Waste Regulatory Analyses (CNWRA) staff. This report summarizes only review activities by the CNWRA staff.

The evaluation focused on verifying the consistency among data, definitions, and algorithms in the SR00_037ne6.gsm file and the supporting DOE documentation. The review was split into two areas, model input and model implementation, consistent with a review outline developed by the NRC staff. For model input verification, a selected sample of data and expressions of the DOE TSPA–GoldSim code was traced to the DOE documentation sources. Similarly, the model implementation activity checked the appropriate function and representation of submodels in the TSPA–GoldSim code with respect to the DOE documentation.

The DOE total system performance assessment submodels reviewed included (i) the radionuclide inventory abstraction, (ii) igneous activity, (iii) waste package and drip shield degradation, (iv) colloid release and transport in the engineered barrier subsystem, and (v) the biosphere model. Submodels (i) and (ii) were reviewed for model input only. Model implementation review activities for submodels (iii), (iv), and (v) included constructing a simplified model to emulate the implementation of the general corrosion model; comparing colloid model verification results in the site recommendation document to outcomes predicted by process model abstraction reports; tracing information flow from the saturated zone model to the biosphere model; and verifying with hand calculations groundwater concentration, water usage, and dose estimates in the biosphere model.

In the inventory abstraction, most radionuclide decay rate values in the SR00_037ne6.gsm file are lower than rates in site recommendation documents. In general, inventory data for DOE-owned spent nuclear fuel and high-level waste in glass form in the inventory vectors of the SR00_037ne6.gsm file deviate significantly from the values cited in the documentation. The latest revision of the inventory abstraction document (Bechtel SAIC Company, 2001) references source data only by title without any data identifier, making it difficult to identify the exact data used in the computations.

For the igneous activity model, complete agreement was found between the SR00_037ne6.gsm file and the DOE documentation for the set of data selected for review.

For the waste package and drip shield degradation models, no documentation was found for the definition of the parameter defining the number of cracks per patch. In addition, there is not enough documentation of an input vector to the general corrosion module. This TSPA–GoldSim code input vector contains more than 1,000 entries, without units or comments, making it difficult to trace any of its values to the DOE documentation. In the model implementation verification activity, a simplified model to emulate the action of the method used by DOE to split distributions of corrosion rates into uncertainty and variability contributions was

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implemented, and adequate agreement with the DOE results was obtained. A simplified approach to emulate the general corrosion abstraction of the DOE TSPA–GoldSim code was implemented. It was not possible to verify that the DOE general corrosion model is consistent with the DOE documentation, because of the significant disagreement between simplified computations and results in the SR00_037ne6.gsm file.

We argue that the fraction of waste packages failed by general corrosion as a function of time depends on the discretization of the waste package surface. There is disagreement between model definitions in the DOE documentation and the actual implementation in the TSPA–GoldSim code. One disagreement pertains to the definition for the fraction of degraded axial length of the waste package. This quantity is used to estimate the amount of water available for radionuclide release. The definition implemented in the TSPA–GoldSim code lacks physical meaning and is not consistent with the documentation. In a second disagreement, the DOE documentation (CRWMS M&O, 2000b) states that the fraction of degraded axial length for the drip shield is used as a factor to estimate the amount of water available for radionuclide release; however, the factor used in TSPA–GoldSim code is the fraction of the surface corroded by general corrosion as a function of time. A plot is presented to assess the effect of the noted inconsistencies. It appears that the approach described in the DOE documentation (CRWMS M&O, 2000 TSPA–SR) is conservative with respect to the approach actually implemented in TSPA–GoldSim code.

There is no clear description, in the documentation, of the relationship between the number of defects from the manufacturing defect abstraction model and the number of cracks from an alternative conceptual model to stress corrosion cracking referred to as the slip dissolution model. Also, there is no documentation on the effect of the discretization size of the waste package surface (i.e., the number of patches) on the size of the area affected by stress corrosion cracking.

To implement colloid release and transport in the engineered barrier subsystem, the majority of reviewed model inputs were correctly represented relative to source documents. One expression showed units mismatch, one data element differed from the DOE documentation, three stochastic elements had different distribution types, and four selector elements differed, at varying degrees, from their source references. In addition, the derivation of two data elements and all six stochastic elements is not transparent. For model implementation, two significant errors were found—one inherited from the supporting DOE documentation and the other failing to implement the abstraction discussed in the documentation. The first implementation error directly affects the calculated mass of iron oxyhydroxide colloids, while the second reflects a failure to implement water mixing in the invert—a model component that can affect the calculated colloid concentrations.

In the DOE biosphere model, no discrepancies were identified between the input data in the TSPA–GoldSim model and the supporting documentation. Model implementation review activities included hand calculations of groundwater concentrations used for dose calculations relevant to individual protection and groundwater protection limits in 10 CFR Part 63 (NRC, 2001). Additional verification checks were performed on concentration calculations related to groundwater protection limits in 10 CFR Part 63. No major problems were identified; however, some aspects of the groundwater protection calculations should be updated for consistency with recently promulgated final regulations in 10 CFR Part 63 (NRC, 2001). Inconsistencies with the final standards include use of a 20-km [12.4-in] compliance boundary, use of the dilution

volume from the proposed standards, use of all pathway biosphere dose conversion factors for the groundwater protection dose calculation, and the lack of an organ dose calculation needed to demonstrate compliance with the groundwater protection dose limit. DOE is planning to incorporate the final regulations into the TSPA–GoldSim code model and supporting documentation in the future.

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1 INTRODUCTION

The U.S. Department of Energy (DOE) is developing a total system performance assessment code intended to support a License Application to construct a geologic repository for disposal of high-level waste at Yucca Mountain, Nevada. The objective of the code is to provide relevant information on the future performance of the repository to support decisions. The DOE total system performance assessment code is being developed using a software tool called GoldSim. GoldSim is a flexible platform for visualizing and dynamically simulating mathematical computations. GoldSim is a visual spreadsheet that allows the graphic creation and manipulation of data and equations. GoldSim is different from common programming languages, such as Fortran, Basic, and C, because the visual interface allows exploration of the model implementation. This interface facilitates traceability of codes developed with the GoldSim platform. In this report, the DOE total system performance assessment code constructed using GoldSim is referred to as the DOE TSPA–GoldSim code or simply the TSPA–GoldSim code.

Results of the TSPA–GoldSim code may be submitted to the U.S. Nuclear Regulatory Commission (NRC) as part of a future License Application for construction of a geologic repository for disposal of high-level waste at Yucca Mountain, Nevada. To prepare for reviewing a License Application, the NRC and Center for Nuclear Waste Regulatory Analyses (CNWRA) staff obtained the TSPA–GoldSim code and conducted a limited review to verify consistency with the DOE documentation and evaluate the adequacy of model implementation and use of data. This report documents the methodology and results of the review by the CNWRA staff. This review is part of a joint effort involving the NRC and CNWRA staffs. It is expected that this report will be part of a broader scope report documenting review results by the NRC and CNWRA staffs in the near future.

1.1 Objective

This report is consistent with review methods described in the Yucca Mountain Review Plan–Draft Report for Comment (NRC, 2002a) concerning the demonstration of compliance with the postclosure individual protection standard. The Yucca Mountain Review Plan (NRC, 2002a) is to ensure the quality, uniformity, and consistency of the NRC staff reviews of any License Application and any amendments. The analysis of repository performance that demonstrates compliance with the postclosure individual protection standard at 10 CFR 63.311 (NRC, 2001) is necessary to ensure DOE has presented an acceptable analysis demonstrating the safety of the repository system. The analysis of repository performance that demonstrates compliance with the postclosure individual protection standard includes the following parts: (i) appropriate incorporation of scenarios into the DOE total system performance assessment results, (ii) calculation of the annual effective dose equivalent from the repository system, and (iii) credibility of the DOE total system performance assessment results. This report focuses on (iii) and is a review of the consistency of information in the DOE documents and the implementation of data, models, and flow of information in the TSPA–GoldSim code. Reviewing the consistency of the information in the TSPA–GoldSim code will aid in developing confidence in the total system performance assessment results.

1.2 Yucca Mountain Review Plan Acceptance Criteria

The Yucca Mountain Review Plan–Draft Report for Comment (NRC, 2002a) provides guidance to evaluate any License Application for the proposed repository at Yucca Mountain. Licensing criteria are specified in 10 CFR Part 63 (NRC, 2001). The U.S. Secretary of Energy recommended the Yucca Mountain site to the President of the United States for development of a nuclear waste repository. The President notified the U.S. Congress that he considers Yucca Mountain qualified for a Construction Permit Application, and the U.S. Congress approved the recommendation (after overriding a veto by the State of Nevada). The DOE is expected to submit a License Application to the NRC. The Yucca Mountain Review Plan will ensure the quality, uniformity, and consistency of NRC staff reviews of any License Application and any amendments. The Yucca Mountain Review Plan has separate sections for reviews of repository safety before permanent closure, repository safety after permanent closure, research and development program to resolve safety questions, performance confirmation program, and administrative and programmatic requirements. Each section supports determining compliance with specific regulatory requirements from 10 CFR Part 63 (NRC, 2001). The particular acceptance criterion in the Yucca Mountain Review Plan—Draft Report for Comment (NRC, 2002a) concerning the Demonstration of Compliance with the Postclosure Individual Protection Standard relevant to this report is presented next.

Acceptance Criterion 3

The Total System Performance Assessment code Provides a Credible Representation of Repository Performance.

- Assumptions made within the total system performance assessment code are consistent among different modules of the code. The use of assumptions and parameter values that differ among modules of the code is adequately documented.

- The total system performance assessment code is properly verified, such that there is confidence that the code is modeling the physical processes in the repository system in the manner intended. The transfer of data between modules of the code is conducted properly.

- The estimate of the uncertainty in the performance assessment results is consistent with the model and parameter uncertainty.

- The total system performance assessment sampling method ensures that sampled parameters have been sampled across their ranges of uncertainty.

1.3 Scope and Content of Report

The evaluation focused on particular submodels of the TSPA–GoldSim code, namely inventory abstraction, igneous activity, waste package and drip shield degradation, colloid release and transport in the engineered barrier subsystem, and biosphere. The review checked the consistency between the information in the TSPA–GoldSim code and the DOE documentation concerning parameter definitions, parameter distributions and values, and model descriptions. The review was split into model input and model implementation. In the model input review,

input data to the code and parameter definitions were traced to source documents. In the model implementation review, the consistency of the action of the TSPA–GoldSim code was evaluated with respect to the model description in the DOE documents. Only model input review was applied to the inventory abstraction because there is no model associated with the inventory data. The igneous activity model was reviewed only with respect to model input, consistent with a review outline elaborated by NRC and tasks assigned to the CNWRA staff. Model input and model implementation reviews were applied to the waste package and drip shield degradation, colloid release and transport in the engineered barrier subsystem, and biosphere models. Positive evaluations in this report in general indicate that information in the TSPA–GoldSim code and the supporting DOE documentation are consistent, that the input data and definitions are in agreement, and that the code performs the functions described in the documentation. Criticism on technical basis and model validity is expressed only in the review of the colloid release and transport in the engineered barrier subsystem model.

This report is structured as follows. Chapter 2 provides a discussion of the review methodology. In Chapter 3, review results are reported. Chapter 3 has been divided into five subsections to discuss (i) inventory abstraction, (ii) igneous activity model, (iii) waste package and drip shield degradation model, (iv) colloid transport, and (v) biosphere model. The content of these five subsections differs because the complexity and model implementation of each aspect in the TSPA–GoldSim model varies. In each of the five subsections, the scope of the review is explicitly defined, and additional information on the review methodology is provided. Model highlights relevant to the review and results of the evaluation concerning model inputs and model implementation are presented in Chapter 3. Chapter 4 summarizes the review.

2 REVIEW APPROACH

An outline presenting a practical approach to review the U.S. Department of Energy (DOE) TSPA—GoldSim code implemented using GoldSim was developed by the U.S. Nuclear Regulatory Commission (NRC) staff prior to beginning review activities. The outline recognizes that a total system performance assessment model is an abstraction that includes selected features, events, and processes believed to be significant to the performance of the system. The NRC review outline includes a sample of the model. If a sample of the total system performance assessment model is well implemented, there is confidence that the complete model is well implemented. The areas of interest of the review task include (i) internal and external model inputs and (ii) model implementation (supporting model confidence-building activities). Center for Nuclear Waste Regulatory Analyses (CNWRA) review activities focused on specific process models pertaining to the inventory abstraction, igneous activity, waste package and drip shield degradation, colloid release and transport in the engineered barrier subsystem, and biosphere model. The inventory abstraction and igneous activity models were only evaluated for (i). Items (i) and (ii) were applied to the evaluation of the remaining submodels reviewed in this report.

NRC obtained from DOE an electronic file generated by the TSPA–GoldSim code. The file, SR00_037ne6.gsm, contains information about a single realization in which each stochastic parameter was fixed at its median value. In this report, checking of the TSPA–GoldSim code means checking the contents of the SR00_037ne6.gsm file. The model input review involved checking a subset of equations and input data values in the SR00_037ne6.gsm file for consistency with supporting documentation. The reviewed documentation includes reports such as the Repository Safety Strategy (CRWMS M&O, 2000a), total system performance assessment documents for the site recommendation (CRWMS M&O, 2000b,c) and various analysis and model reports. The TSPA–GoldSim model includes approximately 800 data elements, 250 stochastic elements, 700 selectors, 650 one-dimensional tables, and 30 two-dimensional tables. Data elements in the GoldSim code are single-value constants (e.g., constants used to specify design dimensions), stochastic elements are parameters defined using distribution functions and sampled from realization to realization, selectors are logic statements, one- and two-dimensional tables are look-up tables that are generally used to interpolate data. The original NRC review outline identified 77 data elements, 56 stochastic elements, 40 selectors, 18 one-dimensional tables, and 4 two-dimensional tables for verification. A subset of these data, representing the portion reviewed by the CNWRA staff, are included in this report.

The NRC outline to perform the review also included examining the use of dynamic link libraries within the TSPA-GoldSim code. Dynamic link libraries are external routines, compiled with independent code languages, such as Fortran, that communicate with TSPA–GoldSim code via input and output files. The structure of the dynamic link libraries cannot be inspected by exploring the TSPA–GoldSim code. It is necessary to check that input and output of information to and from the dynamic link libraries are properly integrated in the TSPA–GoldSim model. For the current review, one subsystem modeled with a dynamic link library (the WAPDEG code developed by the DOE to predict failure of the waste package and drip shield) was evaluated.

The model implementation activity checked appropriate functioning and representation of submodels in the TSPA–GoldSim code against the DOE documentation. The submodels reviewed included waste package and drip shield degradation, colloid release and transport in the engineered barrier subsystem, and bisophere. Model implementation review activities included tracing information flow from the saturated zone model to the biosphere model; verifying with hand calculations groundwater concentration, water usage, and dose estimates in the biosphere model; constructing a simplified model to emulate the implementation of the Gauss-Variance Partitioning method and general corrosion in WAPDEG; and comparing colloid model verification results in (CRWMS M&O, 2000o outcomes predicted by process model abstraction reports. Flexibility in the execution of the review plan is necessary because of differences in the various subsystem models reviewed. Additional details of the particular review activities are available in the main subsections of Chapter 3.

3 SYSTEM-LEVEL MODIFICATION

3.1 Radionuclide Inventory Abstraction

3.1.1 Model Input

Radionuclide inventory abstraction was reviewed for model input only. Because of the simplicity of the abstraction, review of the radionuclide inventory for model implementation is not necessary. The radionuclide inventory is used as input data for release computations. The reviewed data elements of the TSPA–GoldSim code in the SR00_037ne6.gsm file pertinent to the radionuclide inventory abstraction are summarized in Table 3-1.

The inventory abstraction document (CRWMS M&O, 2000d)) and supporting site recommendation computations (CRWMS M&O, 2000b) references decay rate values from Walker, et al. (1984) in calculations of the average commercial spent nuclear fuel, DOE-owned spent nuclear fuel, and high-level waste inventories in commercial spent nuclear fuel and codisposal waste packages. Input from the source data (CRWMS M&O, 2000e) is used in the inventory abstraction document (CRWMS M&O, 2000d) for radionuclide screening analysis. For verification purposes of the radionuclide decay rate values in the DOE calculations, source data titled Relative Contribution of Individual Radionuclides to Inhalation and Ingestion Dose; Ten Thousand Years (data identifier SN9910T08110599.001), which exist only in electronic form, was requested from DOE. Apparently this source data is no longer available and has been superseded by source data with data identifier SN0012T0810599.039 of the same title, provided by DOE on a compact disk following the request by the U.S. Nuclear Regulatory Commission. The source data indicate the website http://www.dne.bnl.gov/CoN/index.html as reference for decay rate values, which differs from the reference (Walker, et al., 1984) of the inventory abstraction document (CRWMS M&O, 2000d). This website readdresses visitors to http://www2.bnl.gov/ton/ where an interactive Table of Nuclides is implemented (copyrighted by the Nuclear Data Evaluation Laboratory of the Korean Atomic Energy Research Institute). Therefore, half-life values from this latter website were used to derive decay rates for comparison with the TSPA–GoldSim SR00_037ne6.gsm file. The latest revision of the inventory abstraction document (Bechtel SAIC Company, 2001) references the source data only by its title (i.e., Relative Contribution of Individual Radionuclides to Inhalation and Ingestion Dose; Ten Thousand Years), without any data identifier. Therefore, it is not clear if data used in Bechtel SAIC Company (2001) indeed supersede data referenced by site recommendation analyses in CRWMS M&O (2000b). The TSPA–GoldSim SR00_037ne6.gsm file references Lide (1991–92) for half-life data.

The source data decay rate values for 26 radionuclides considered in the inventory model reported in CRWMS M&O (2000b) were compared with the Decay_Rate data vectors in the TSPA–GoldSim SR00_037ne6.gsm file. All decay rate deviations are within 2 percent for all radionuclides except I-129 (7.7 percent). Decay rate values used in the source data (CRWMS M&O, 2000e) agree with the corresponding values derived from half-lives from the website http://www2.bnl.gov/ton/ except for Th-229 (7 percent difference). Decay rate values used in the TSPA–GoldSim SR00_037ne6.gsm file agree with the data from Lide, 1991–92.

Table 3-1. Reviewed TSPA–GoldSim Code Data Related to the Radionuclide Inventory Abstraction	
Data	**References**
Decay_Rate	CRWMS M&O, b,d; Walker, et al., 1984; Lide, 1991–92; Source Data: SN9910T0810599.001; Source Data: SN0012T0810599.039; http://www.dne.bnl.gov/CoN/index.html *
CSNF_Inventory	CRWMS M&O, 2000b,d
DSNF_Inventory	CRWMS M&O, 2000b
HLW_Inventory	CRWMS M&O, 2000b
Total_CSNF_packages	CRWMS M&O, 2000b
*Website referenced in the Source Data website readdresses visitors to http://www.2.bnl.gov/ton/	

Commercial spent nuclear fuel inventory data contained in GoldSim CSNF_Inventory data vector are in agreement with data in CRWMS M&O (2000b). Inventory data for Am-241 in CRWMS M&O (2000b) report a value of 1.09×10^4 g/pkg [24 lb/pkg], while the inventory abstraction document (CRWMS M&O, 2000d), referenced as source of data and its subsequent revision Bechtel SAIC Company (2001) report a value 8.76×10^3 g/pkg [19.3 lb/pkg] for Am-241.

DOE-owned spent nuclear fuel inventory data were compared with data reported in CRWMS M&O (2000b). Inventory ratios of TSPA-GoldSim versus values in CRWMS M&O (2000b) range from 0.63 to 16.51. The same ratios for 13 radionuclides range from 0.63 to 1; 3 ratios are in the 1 to 2 range, and 10 ratios lie between 2 and 16.51. For radionuclides with inventory ratios below unity, 12 ratios are within 10 percent of the values in CRWMS M&O (2000b) [e.g., the value for U-236 is 0.63 of the value in CRWMS M&O (2000b)]. For Np-237, I-129, and Tc-99 the ratios are 8.9, 3.22, and 3.94. Detailed comparison results are presented in Figure 3-1.

High-level waste glass inventory data in the SR00_037ne6.gsm file were compared with the data in CRWMS M&O (2000b). Ratios of TSPA–GoldSim and data in CRWMS M&O (2000b) range from 0.02 to 3.01; the ratios for 20 radionuclides are within the 0.002 to 1 range, and for 6 radionuclides, within the 1 to 3.01 range. Detailed comparisons are presented in Figure 3-2. Figure 3-2(b) presents a comparison for ratios in the less than unity range.

The input value for mass of surrogate colloidal species in TSPA-GoldSim inventory data vectors is 10^6 g/package [2,205 lb/package] for high-level waste packages and zero for packages containing commercial spent nuclear fuel and DOE-owned spent nuclear fuel. In CRWMS M&O (2000b), the colloidal concentration was defined as a function of ionic strength for all three waste forms, presented in units of mass per volume (mg/L), and cites an arbitrary large value (CRWMS M&O, 2000b), for the initial value of surrogate colloidal species in the glass waste form cell. Therefore, direct comparison of colloidal species inventory data in the

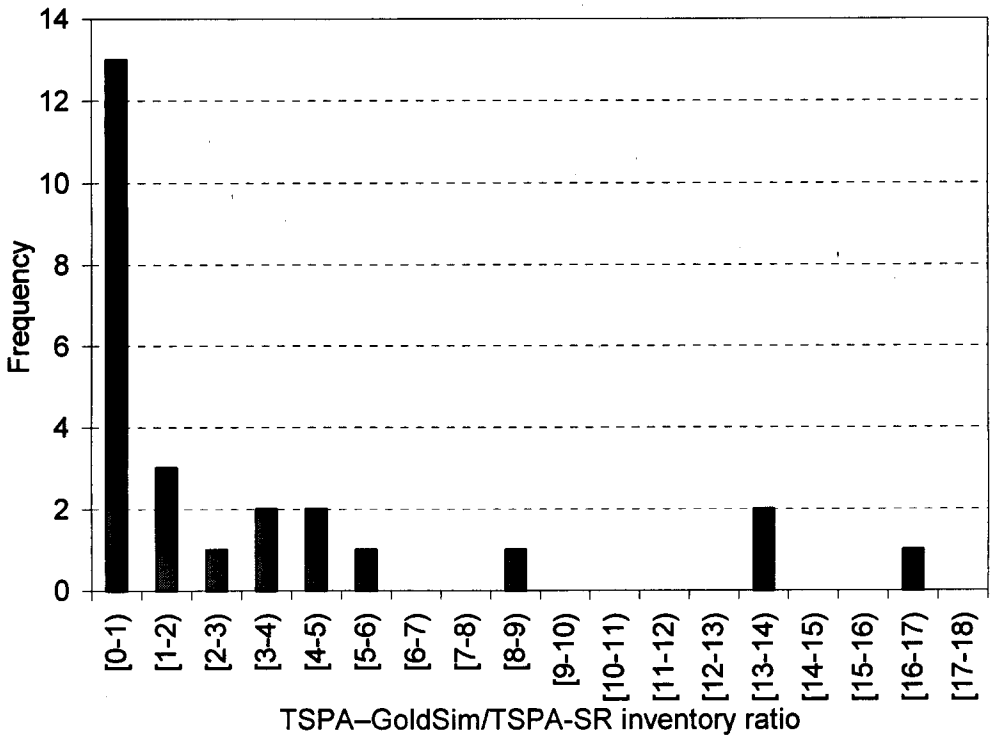

Figure 3-1. Frequency of Occurrence of Ratios of TSPA–GoldSim and Inventory data for 26 Radionuclides Considered in the Site Recommendation Model (CRWMS M&O, 2000b) for DOE-owned Spent Nuclear Fuel in Codisposal Waste Package (mass per package, g/package).

SR00_037ne6.gsm file and in CRWMS M&O (2000b) is not feasible. In the site recommendation model, commercial spent nuclear fuel was assumed not to produce colloids; however, commercial spent nuclear fuel radionuclides can reversibly attach to naturally occurring colloids and to corrosion-product colloids. In the inventory data vector in the SR00_037ne6.gsm file, the colloidal species is considered only for high-level waste glass. The total number of commercial spent nuclear fuel waste packages in the TSPA-GoldSim code, Total_CSNF_packages, is in agreement with CRWMS M&O (2000b).

In conclusion, most radionuclide decay rates in the TSPA-GoldSim SR00_037ne6.gsm file are generally lower than rates referenced in the site recommendation document (CRWMS M&O, 2000b). Inventory data for DOE-owned spent nuclear fuel and high-level waste contained in the TSPA-GoldSim code inventory data vectors deviate significantly from the values in CRWMS M&O (2000b).

3.2 Igneous Activity

Review tasks assigned to CNWRA staff were restricted to model input only. This section will be expanded when NRC reviews are incorporated into the report.

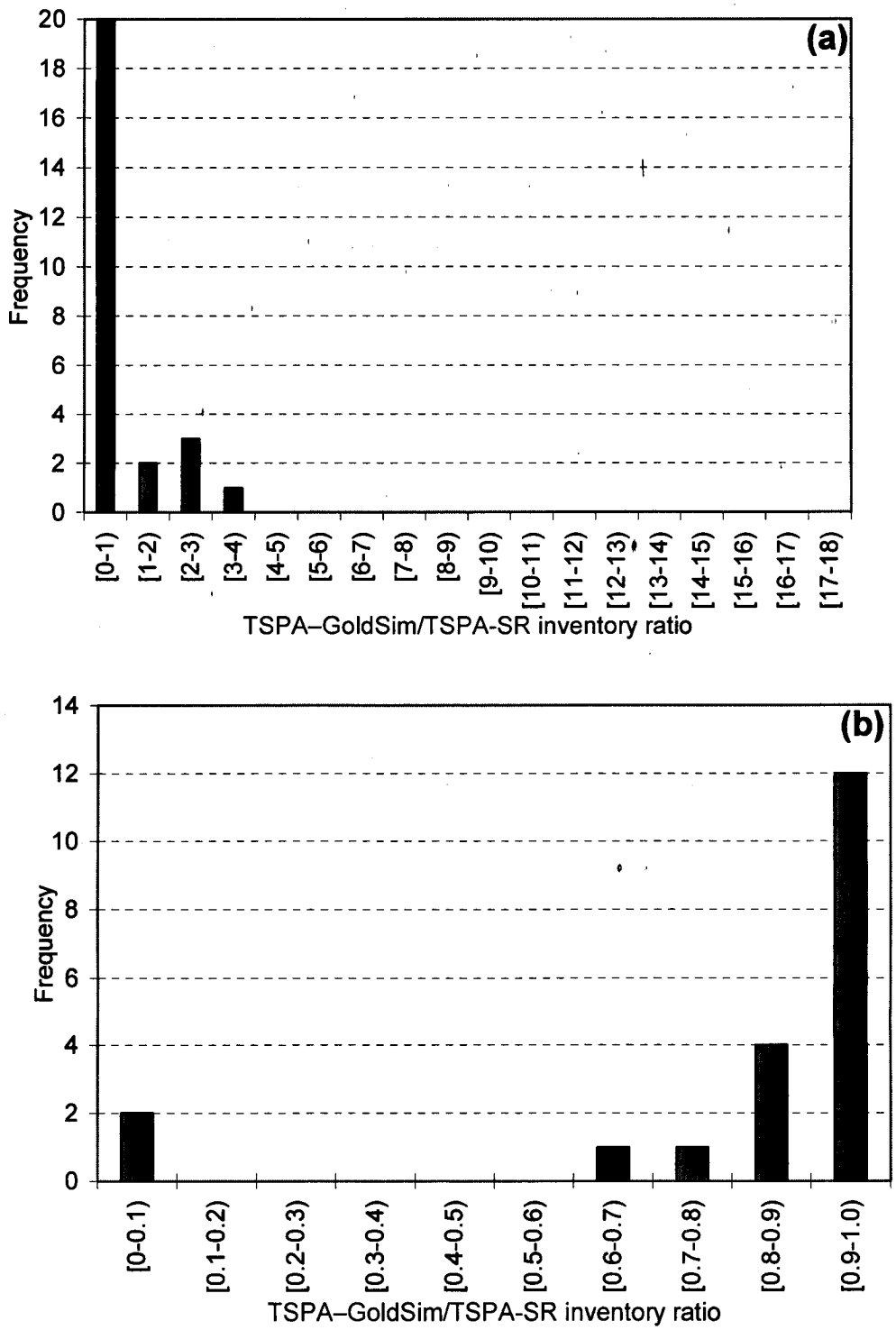

Figure 3-2. Frequency of occurrence of ratios of TSPA–GoldSim and inventory data for 26 radionuclides considered in the site recommendation model (CRWMS M&O, 2000b) for high-level waste in a codisposal waste package (mass per package, g/package); (a) ratios in the complete range; (b) ratios in the 0–1 range.

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Table 3-2. TSPA–GoldSim Variables Related to Igneous Activity	
Expressions	**References**
Ash_Dose	CRWMS M&O, 2000c
Weight_Ash_Dose	CRWMS M&O, 2000c
Total_Ash_Dose	CRWMS M&O, 2000c
Num_Pkgs_Hit	CRWMS M&O, 2000b,c,f
CSNF_Hit	CRWMS M&O, 2000c
Event_Probability	CRWMS M&O, 2000b,c,f
Data	**References**
HLW_Ash_Inventory	CRWMS M&O, 2000c
BDCF_Ash_	CRWMS M&O, 1999, 2000b,c
Ashden_Min	CRWMS M&O, 2000c,f
Ashden_Max	CRWMS M&O, 2000c,f
denash	CRWMS M&O, 2000c,f
Stochastic	**References**
Vent_Diameter	CRWMS M&O, 2000c,f
NVents	CRWMS M&O, 2000c
Soil_Removal	CRWMS M&O, 2000c
Erupt_Volume	CRWMS M&O, 2000b,c,f
Power	CRWMS M&O, 2000b,c,f
Erupt_Velocity	CRWMS M&O, 2000b,c,f
u	CRWMS M&O, 2000b,c,f

3.2.1 Model Input

The reviewed expressions, data, and stochastic data of the TSPA–GoldSim code pertinent to igneous activity models are summarized in Table 3-2. The TSPA–GoldSim code variables reviewed represent only a cross section of those used in the igneous activity model. A sample review would yield information supporting the consistency of the model implementation with respect to the DOE documentation. All 18 expressions, data, and stochastic elements of the TSPA–GoldSim code SR00_037ne6.gsm file were consistent with the DOE documentation. The consulted DOE documentation included four CRWMS M&O reports (1999, 2000b,c,f).

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3.3 Waste Package and Drip Shield Degradation

3.3.1 Model Input

The reviewed expressions, data, and stochastic elements of the TSPA–GoldSim code pertinent to the waste package and drip shield degradation models are summarized in Table 3-3. In general, adequate agreement was found between the definitions and values in the SR00_037ne6.gsm file and in the DOE documentation. No explicit reference to the parameter Cracks_per_Patch_Factor was found in CRWMS M&O (2000b,c,g). The parameter, Cracks_per_Patch_Factor, is used to compute the area affected by stress corrosion cracking—later used to determine the extent of diffusive radionuclide release. Also, there is insufficient information on the meaning of the entries of the vector WAPDEG_inputs. This vector is used as input to the WAPDEG dynamic link library to compute failure times and the degradation extent of the drip shield and waste package. The vector, WAPDEG_inputs, contains more than 1,000 entries. No descriptive information is available in the TSPA–GoldSim code environment, and no documentation is available explaining each of the entries of the vector. Therefore, judgment cannot be made on adequacy of the information in the WAPDEG_inputs vector.

3.3.2 Model Implementation

3.3.2.1 Scope of Review

This section reviews the computation of waste package and drip shield degradations by general corrosion and stress corrosion cracking of the closure weld area of the waste package. Also, reviewed in the Gauss-Variance Partitioning algorithm, which is used to perform differentiation between variability and uncertainty in the variance of the corrosion rates. The module of the total system performance assessment model performing the drip shield and waste package degradation computations is known as WAPDEG, which has been implemented in the form of dynamic link library independent of the TSPA–GoldSim code. The WAPDEG dynamic link library communicates with the TSPA–GoldSim code via input and output files. Therefore, the structure of the WAPDEG code cannot be reviewed by browsing the TSPA–GoldSim SR00_037ne6.gsm file. Simplified computations were performed to verify the implementation of the Gauss-Variance Partitioning method and general corrosion in WAPDEG, and the results are discussed.

3.3.2.2 Model Highlights

The main output of the model for the degradation of the drip shield and waste package is the extent of the degradation of the surface as a function of time. An estimate of the degradation that ranges from 0 to 1 (0 means no degradation and 1 means complete degradation) is computed by WAPDEG, which is then used as a factor to estimate the amount of water available for advective release of radionuclides. In the case of stress corrosion cracking of the closure weld of the waste package, the main output of the model is the size of the surface affected by cracks, for each waste package, as a function of time. This surface area is used downstream in the total system performance assessment model to compute the extent of diffusive release of radionuclides.

Table 3-3. TSPA–GoldSim Code Variables Related to Waste Package and Drip Shield Degradation	
Expressions	**References**
WP_Total_Patch_Area_CSNF	CRWMS M&O, 2000c
WP_Total_Crack_Area	CRWMS M&O, 2000c
ASCCib	CRWMS M&O, 2000c,g
ASCCob	CRWMS M&O, 2000c,g
WP_SA_CDSP	CRWMS M&O, 2000c
WP_SA_CSNF	CRWMS M&O, 2000c
Data	**References**
Cracks_per_Patch_Factor	No reference available
WAPDEG_inputs	CRWMS M&O, 2000c,g
MFD_middle_lid\lid_radius	CRWMS M&O, 2000c,g
MFD_outer_lid\lid_radius	CRWMS M&O, 2000c,g
A1_OL	CRWMS M&O, 2000c,g
A2_OL	CRWMS M&O, 2000c,g
A3_OL	CRWMS M&O, 2000c,g
A4_OL	CRWMS M&O, 2000c,g
nangle	CRWMS M&O, 2000c,g
YS_OL	CRWMS M&O, 2000c,g
fys_OL	CRWMS M&O, 2000c,g
amp_OL	CRWMS M&O, 2000c,g
Length_CSNF	CRWMS M&O, 2000c,h
Radius_CSNF	CRWMS M&O, 2000c,h
Thick_WP	CRWMS M&O, 2000c,h
WP_Patch_Area_CSNF	CRWMS M&O, 2000c
Number_DS_Patches	CRWMS M&O, 2000c
Stochastic	**References**
u_GVP_GA22SR00	CRWMS M&O, 2000c
qu_ GVP_GA22SR00	CRWMS M&O, 2000c
b_ML	CRWMS M&O, 2000c,g
v_ML	CRWMS M&O, 2000c,g

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Table 3-3. TSPA–GoldSim CodeVariables Related to Waste Package and Drip Shield Degradations (continued)	
psi_ML	CRWMS M&O, 2000c,g
Expressions	**References**
b_OL	CRWMS M&O, 2000c,g
v_OL	CRWMS M&O, 2000c,g
psi_OL	CRWMS M&O, 2000c,g
nib	CRWMS M&O, 2000c,g
nob	CRWMS M&O, 2000c,g
z_OL	CRWMS M&O, 2000c,g
stress_threshOLfac	CRWMS M&O, 2000c,g

The degradation modes of the drip shield considered in the total system performance assessment model are general corrosion and hydrogen-induced cracking, however, general corrosion is the dominant degradation mode according to documented results (CRWMS M&O, 2000b). Conceptualizations for general corrosion, microbial corrosion, thermal aging, localized corrosion, and stress corrosion cracking of the waste package are also available in the total system performance assessment model. Although a model for localized corrosion is available in WAPDEG, localized corrosion is practically screened out from the total calculations because the experimental database supporting the model causes that the mathematical conditions leading to activation of localized corrosion within WAPDEG are never met. Microbially influenced corrosion and thermal aging are modeled in total system performance assessment by enhancement factors to the general corrosion rate. Thermal aging and stress corrosion cracking are assumed to affect only the closure-weld area. Therefore, the most important aspects of the WAPDEG implementation are general corrosion and stress corrosion cracking. Furthermore, implementation of stress corrosion cracking is linked to the general corrosion model because, for stress corrosion cracking to occur, a predefined thickness of the closure weld must be corroded away by general corrosion. Therefore, general corrosion was reviewed in detail. Additional details on the total system performance assessment modeling of general corrosion and stress corrosion cracking are provided in Subsections 3.3.2.3.2.1 and 3.3.2.3.3.

3.3.2.3 Review Findings

3.3.2.3.1 Gauss-Variance Partitioning Method

A detailed analysis of the Gauss-Variance Partitioning method was performed. The DOE documentation on the Gauss-Variance Partitioning is brief and not sufficient to develop an intuition on the effect of the method to separate a distribution into multiple components (referred to by the DOE as uncertainty and variability components). The effect of the Gauss-Variance Partitioning on extreme values of distributions of corrosion rates may be important, because the highest corrosion rates determine failure times of drip shields and waste packages. The detailed analyses indicate that frequency of sampling corrosion rates is not altered by the Gauss-Variance Partitioning method. Details of the review are provided next.

The Gauss-Variance Partitioning method is implemented in the WAPDEG code to split distributions into uncertainty and variability components to support Monte Carlo analyses of relevant output data. Although the Gauss-Variance Partitioning method can be applied to any distribution, in WAPDEG it is mainly used on the distribution of corrosion rates (of Alloy 22 and Titanium Grade 7). Within a single realization of the Monte Carlo implementation, corrosion rates are sampled from a particular component of the original distribution of rates, referred to as the variability distribution. Variability distributions vary from realization to realization because of uncertainty. In other words, DOE adopted an operational definition for variability and uncertainty in the corrosion rates: variation in the corrosion rate within a realization is due to variability and variations of the distribution of corrosion rates from realization to realization are due to uncertainty. The objectives of this section are to explore the theoretical basis behind the Gauss-Variance Partitioning method and to explore characteristics of the variability-uncertainty split to develop an informed intuition on the effect of the method.

3.3.2.3.1.1 Notation

Some mathematical terms are defined to facilitate discussion.

Normal probability density function (mean = μ, and standard deviation = σ):

$$f_{\mu,\sigma}(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \tag{3-1}$$

Normal cumulative density function (mean = μ, and standard deviation = σ):

$$F_{\mu,\sigma}(x) = \int_{-\infty}^{x} f_{\mu,\sigma}(t)dt = \frac{1}{2}\left[1 + \mathrm{erf}\left(\frac{x-\mu}{\sigma\sqrt{2}}\right)\right] \tag{3-2}$$

where erf is the error function defined as

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt \tag{3-3}$$

In Subsections 3.3.2.3.1.1 and 3.3.2.3.1.2, cumulative distribution functions are denoted with uppercase letters [e.g., $F_{\mu,\sigma}(x)$], and probability distribution functions are denoted with lowercase letters [e.g., $f_{\mu,\sigma}(x)$]. By definition $dF_{\mu,\sigma}/dx = f_{\mu,\sigma}(x)$.

The convolution of two functions, f and g, is defined as

$$f * g(x) = \int_{-\infty}^{\infty} f(t)g(x-t)dt = \int_{-\infty}^{\infty} f(x-t)g(t)dt \tag{3-4}$$

where f and g are assumed to be integrable functions.

3.3.2.3.1.2 Discussion

Gauss-Variance Partitioning method depends on a property of the normal distribution: the convolution of two normal probability density functions results in a normal probability density function, that is

$$f_{\mu_1,\sigma_1} * f_{\mu_2,\sigma_2}(x) = f_{\mu_1+\mu_2,\sqrt{\sigma_1^2+\sigma_2^2}}(x) \tag{3-5}$$

If the standard deviations σ_u and σ_v are selected such that

$$\sigma_u^2 + \sigma_v^2 = \sigma^2 \tag{3-6}$$

then, the normal probability density function, $f_{\mu,\sigma}$, can be expressed as a convolution:

$$f_{\mu,\sigma}(x) = f_{\mu,\sigma_u} * f_{0,\mu_v}(x) = \int_{-\infty}^{\infty} f_{\mu,\sigma_u}(m) f_{0,\sigma_v}(x-m)\mathrm{d}m \tag{3-7}$$

By direct substitution it can be verified that $f_{0,\sigma_v}(x-m) = f_{m,\sigma_v}(x)$. This relationship is the core of the Gauss-Variance Partitioning method. From Eq. (3-7), the Gauss-Variance Partitioning algorithm is derived to perform the variability-uncertainty split of a normal distribution $f_{\mu,\sigma}$:

$$f_{\mu,\sigma}(x) = \int_{-\infty}^{\infty} f_{\mu,\sigma_u}(m) f_{m,\sigma_v}(x)\mathrm{d}m \tag{3-8}$$

Step 1) Sample "centers" m from the distribution f_{μ,σ_u}

Step 2) Construct distributions f_{m,σ_v} around each center m

Step 3) Sample the same number of points from each of the derived distributions f_{m,σ_v}

Step 4) Gather all sampled data into a single set.

The population of data derived after Step 4 has $f_{\mu,\sigma}$ as its probability density function in the limit when sufficient centers and sufficiently large data sets are sampled. The deviations σ_u and σ_v are referred to by the DOE as the uncertainty and variability components of the total standard deviation, σ. DOE has adopted the following definition for σ_u and σ_v:

$$\sigma_u^2 = \eta\sigma^2 \tag{3-9}$$

$$\sigma_v^2 = (1-\eta)\sigma^2 \tag{3-10}$$

where $0 \le \eta \le 1$ (with such definition it is ensured that $\sigma^2 = \sigma_u^2 + \sigma_v^2$). A system decomposed according to Eq. (3-9) and (3-10) is referred to by the DOE as containing $\eta \times 100$-percent uncertainty and $(1-\eta) \times 100$-percent variability. Figure 3-3 displays examples of data sets derived using the Gauss-Variance Partitioning method (summarized in Steps 1–4) with three combinations of the uncertainty-variability split of a normal distribution with mean, $\mu = 6$, and standard deviation, $\sigma = 1$. The grey lines in the background of the three plots in Figure 3-3 are referred to as the variability distributions. In a plot, all variability distributions have the same standard deviation, σ_v. The variability distributions are broadly spread if the value of the uncertainty standard deviation, σ_u, is large [e.g., Figure 3-3(a)] and narrowly spread if σ_u is

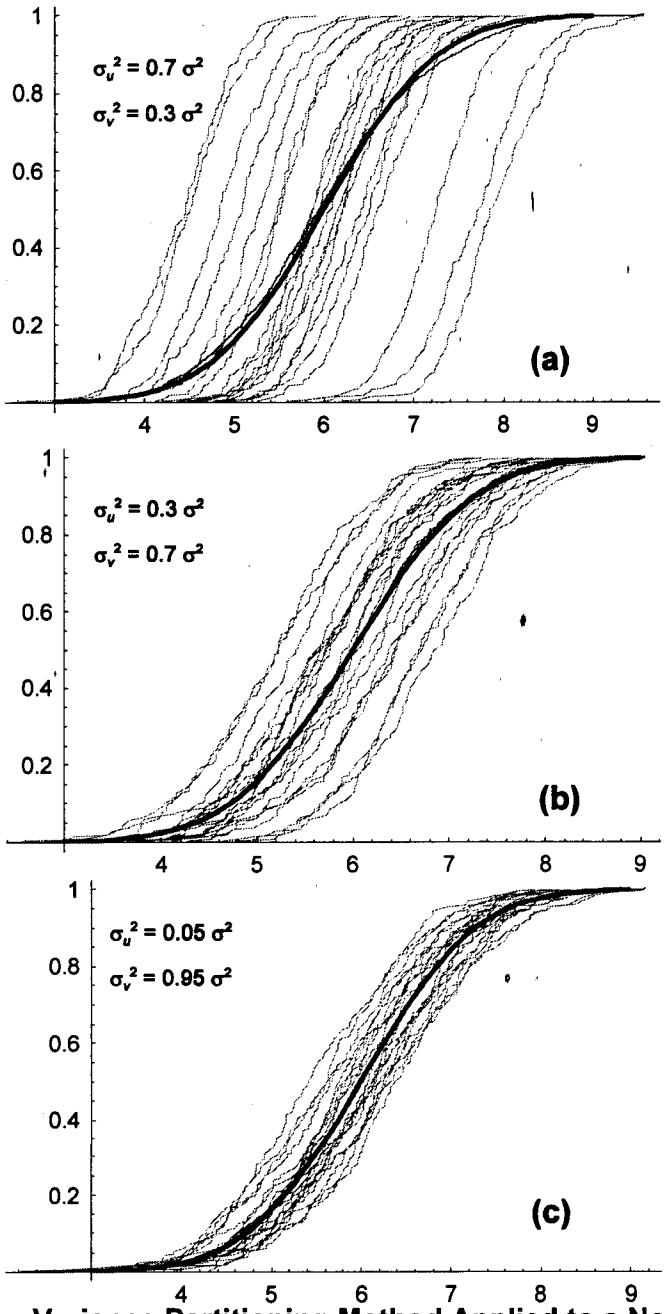

Figure 3-3. Gauss-Variance Partitioning Method Applied to a Normal Distribution (Mean = 6, Standard Deviation = 1) with 3 Combinations of the Uncertainty-Variability Split: (a) 70-Percent Uncertainty and 30-Percent Variability, (B) 30-Percent Uncertainty and 70-Percent Variability, and (C) 5-Percent Uncertainty and 95-Percent Variability. The standard deviation of the variability distributions (background grey lines) equals σ_v. The centers (median values) of the variability distributions are normally distributed with mean = 6 and standard deviation = σ_u. The dark thin line was derived by gathering the samples of the variability distributions into a single population set and computing the corresponding discrete cumulative distribution function. The thick line is the expected theoretical normal cumulative distribution function (mean = 6 and variance = 1).

small [e.g., Figure 3-3(c)]. In the limit, $\sigma_u = 0$, all variability distributions overlap to the original distribution. On the other hand, in the limit, $\sigma_v = 0$, the variability cumulative distributions converge to step functions, normally distributed in the plane.

The Gauss-Variance Partitioning method can be extended to any arbitrary distribution. The modification to the algorithm is explained next. Let x be a stochastic variable with a probability density function denoted as g and a cumulative density function denoted as G [necessarily $dG/d(x) = g(x)$]. The x-space can be mapped into a y-space normally distributed by the following mapping:

$$y = F_{0,1}^{-1}\big(G(x)\big) = F_{0,1}^{-1} \circ G(x) = Y(x) \tag{3-11}$$

The mapping function Y is defined as $Y = F_{0,1}^{-1} \circ G$. Thus, the stochastic variable, y, is normally distributed with $\mu = 0$ and $\sigma = 1$. The Gauss-Variance Partitioning algorithm described previously can be applied to derive variability-uncertainty partitions in the y-space. After the derivation of the partitions, the y-space is mapped back to the x-space by the function

$$x = G^{-1}\big(F_{0,1}(y)\big) = G^{-1} \circ F_{0,1}(y) = X(y) \tag{3-12}$$

The mapping function X is defined as $X = G^{-1} \circ F_{0,1}$ (evidently, $X = Y^{-1}$).

This is a summary of the generalized Gauss-Variance Partitioning algorithm:

Step 1) Define the cumulative density function, $G(x)$, and the probability density function, $g(x)$
Step 2) Map the x-space into the y-space: $y = Y(x)$
Step 3) Determine the extent of the variability-uncertainty partition: $\sigma_u^2 = \eta$, $\sigma_v^2 = 1-\eta$
Step 4) Sample the centers, m, from f_{0,σ_u}
Step 5) Draw random populations from the variability distributions f_{m,σ_v}
Step 6) Map each variability population in the y-space, derived in Step 5, into variability populations in the x-space by use of the mapping $x = X(y)$
Step 7) Collapse all variability populations in the x-space into a single population

It can be rigorously proven that the data population derived after Step 7 has a probability density function equal to the original distribution, g. It is intuitively clear that the original distribution, g, must be recovered after the completion of the algorithm because the X and Y functions are complete mappings. Examples are presented in Figures 3-4 and 3-5 of the Gauss-Variance Partitioning method applied to the uniform and lognormal distributions.

Figures 3-4 and 3-5 display similar trends to those observed in Figure 3-3: the spread of the variability distributions decreases with decreasing values of σ_u. In the limit, $\sigma_u = 0$, all variability distributions overlap to the originating distribution. Note that all derived variability distributions (the grey lines in Figures 3-4 and 3-5) contain the extremes of the original distribution. For example, the uniform distribution in Figure 3-4 is bounded between 0 and 10,

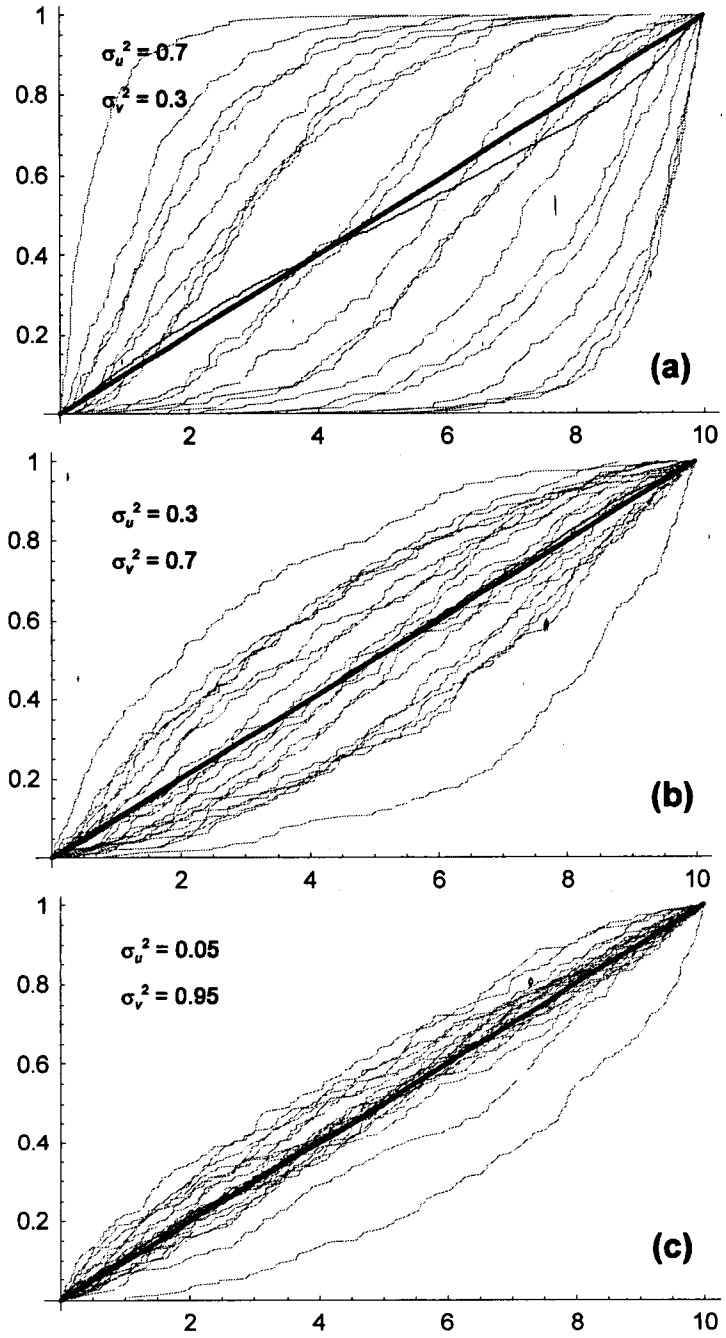

Figure 3-4. Gauss-Variance Partitioning Method Applied to a Uniform Distribution (Extremes: 0 and 10) with 3 Combinations of the Uncertainty-Variability Split: (a) 70-Percent Uncertainty and 30-Percent Variability, (b) 30-Percent Uncertainty and 70-Percent Variability, and (c) 5-Percent Uncertainty and 95-Percent Variability. The Background Grey Lines Are the Derived Variability Distributions. The Dark Thin Line was Derived by Gathering the Samples of the Variability Distributions into a Single population Set and Computing the Corresponding Discrete Cumulative Distribution function. The Thick Line Is the Expected Theoretical Uniform Cumulative distribution Function.

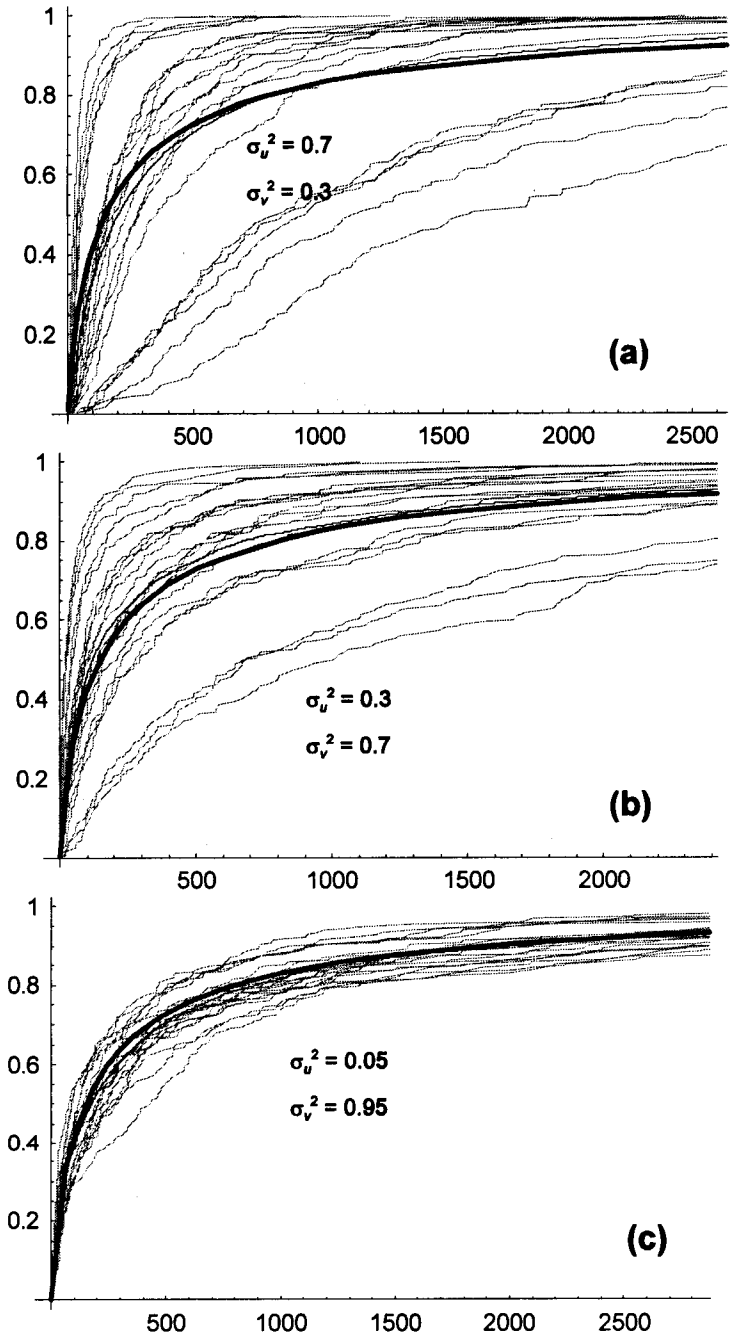

Figure 3-5. Gauss-Variance Partitioning Method Applied to a Lognormal Distribution with 3 Combinations of the Uncertainty-Variability Split: (a) 70 Percent-Uncertainty and 30-Percent Variability, (b) 30-Percent Uncertainty and 70-Percent Variability, and (c) 5-Percent Uncertainty and 95-Percent Variability. The Background Grey Lines Are the derived Variability Distributions. The Dark Thin Line Was Derived by Gathering the Samples of the Variability Distributions into a Single Population Set and Computing the Corresponding Discrete Cumulative Distribution Function. The Thick Line Is the Expected Theoretical Lognormal Cumulative Distribution Function (Mean and Standard Deviations in a Log Space: 5 and 2).

and all subdistributions in Figure 3-4 share exactly the same extreme values (0 and 10). The lower bound of the log-uniform distribution in Figure 3-3 is zero, and it is evident that all derived distributions have the same lower bound. The property that the originating distribution and the derived variability distributions by the Gauss-Variance Partitioning method share identical extreme values can be demonstrated to be valid in general. This property is important because it allows *a priori* identification of the maximum and minimum attainable values of the variability distributions derived by the Gauss-Variance Partitioning method, in the limit when the population size of sampled values tends to infinity. The maximum considered corrosion rate for Alloy 22 is 73 nm/yr [2.87×10^{-6} in/yr] (CRWMS M&O, 2000i), and this maximum value determines the earliest possible failure time of a patch on the waste package (the definition of patch is provided in Section 3.3.2.3.2.1). This maximum rate must be part of any large enough population of corrosion rates.

Given the fact that the proportion of the variability-uncertainty split [i.e., the value of η in Eq. (3-9) and (3-10)] is itself uncertain, DOE opted to sample the fraction η uniformly in the range (0,1). Intuitively, this additional sampling step must not alter the shape of the reconstructed distribution. This statement can be verified graphically and can be rigorously proven. The effect of the sampling of η and the Gauss-Variance Partitioning method is explored in a normal distribution with $\mu = 0$ and $\sigma = 1$. Equations (3-11) and (3-12) guarantee that if the reconstructed distribution coincides with the originating normal distribution, the procedure is also successful when extended to any arbitrary distribution.

From Figure 3-6 it is evident that the original normal distribution is reconstructed. The main visual difference between Figures 3-3 and 3-6 is the crossing of the variability distributions (grey lines) in the latter figure. The crossing is a direct consequence of the sampling of the fraction η, resulting in multiple values of σ_v (in Figure 3-3, single values of σ_v are displayed). Therefore, it can be concluded that the original distribution is reconstructed by the Gauss-Variance Partitioning method when the variability-uncertainty fraction, η is sampled.

In conclusion, the Gauss-Variance Partitioning technique is a method to decompose a distribution into multiple distributions without creating additional information. The proposed operational definition of uncertainty and variability by DOE is reasonable. There is no evident reason why the split should affect Monte Carlo results, especially given the uniform sampling of the variability-uncertainty partition fraction. It is conjectured, however, that the Gauss-Variance Partitioning split expedites the convergence of mean values of relevant output data of the Monte Carlo analysis. For implementation of the Gauss-Variance Partitioning method in WAPDEG, the authors consulted the documentation available in (CRWMS M&O, 2000g,i). A Gauss-Variance Partitioning subroutine was developed in Fortran 90 to support the WAPDEG code, and its outcome was compared to a simple implementation of the Gauss-Variance Partitioning algorithm in Mathcad. Output data from both implementations compared well. The Mathcad function is similar to the Mathematica® implementation used to construct Figures 3-3 to 3-6. The Gauss-Variance Partitioning Fortran subroutine allows a logarithmic transformation of the input population before computing the variability-uncertainty split. The output uncertainty-variability populations are mapped back to the original space by applying the exponential function. This log-transform option is not used in a default run of the WAPDEG code as part of the TSPA–GoldSim code. Based on a review of the documentation, we conclude that the Gauss-Variance Partitioning subroutine of the WAPDEG code is well implemented.

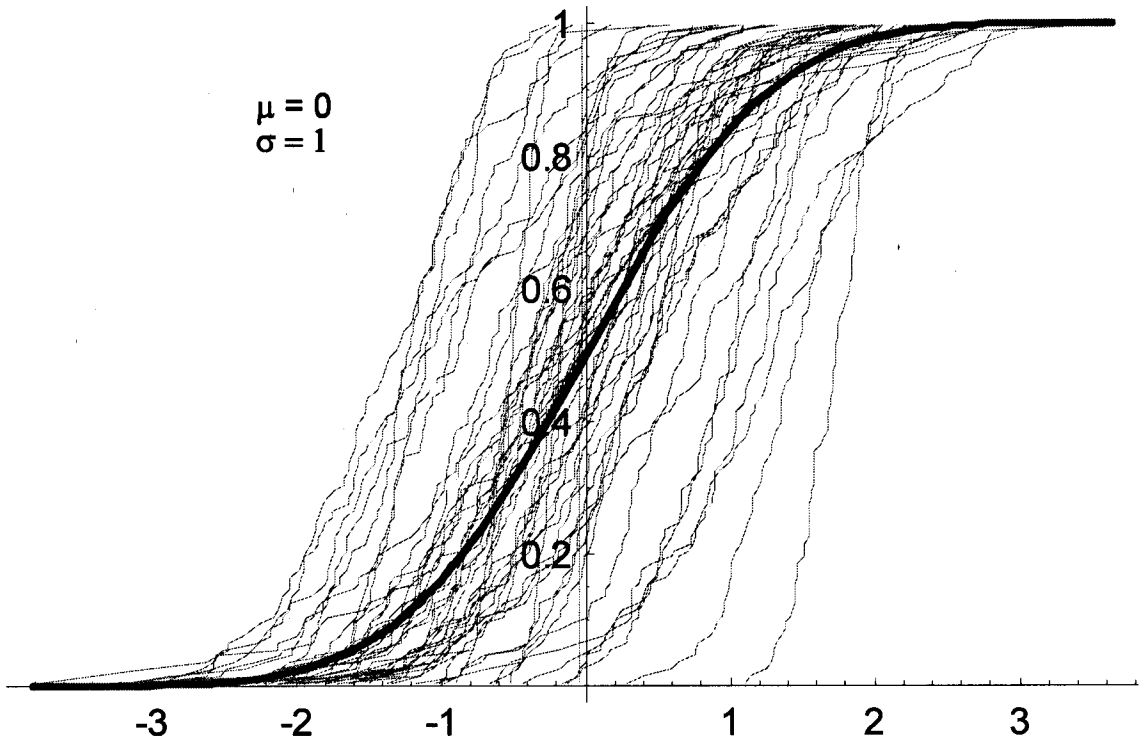

Figure 3-6. Gauss-Variance Partitioning method applied to a normal distribution ($\mu = 0$, $\sigma = 1$) sampling the variability-uncertainty split fraction uniformly in the range (0,1). The background grey lines are the derived variability distributions. The dark thin line was derived by gathering the samples of the variability distributions into a single population set and computing the corresponding discrete cumulative distribution function. The thick line is the expected theoretical normal cumulative distribution function.

Besides, our independent computations to reproduce input data for the TSPA–GoldSim code median case (SR00_037ne6.gsm file) compare well (see Figure 3-8).

3.3.2.3.2 General Corrosion

An external dynamic link library containing an implementation of the WAPDEG code is invoked by TSPA–GoldSim code to compute waste package and drip shield failure times. The dynamic link library implementation does not allow checking the structure of the WAPDEG code by browsing the SR00_037ne6.gsm file . The general corrosion computations within WAPDEG, however can be simplified and implemented in a scientific software such as Mathematica®. The result of the simplified Mathematica® routine can be compared to the median value TSPA–GoldSim code results in the SR00_037ne6.gsm file or results reported in the DOE documents (e.g., CRWMS M&O, 2000b). A simple implementation facilitates efficient inquiring of convergence issues such as the minimum discretization of the waste package surface necessary to guarantee convergence of the fraction of failed surface versus time. In this

section, the general corrosion implementation in WAPDEG is investigated with a more simplified routine developed in Mathematica®, and important convergence questions are addressed. For brevity, the analysis focuses on the general corrosion of the waste package, although a similar analysis could be accomplished for the general corrosion of the drip shield.

Alloy 22 general corrosion rates measured during a 2-year period under a variety of chemical conditions (simulated dilute, simulated concentrated, and simulated acidic waters in the laboratory), exposures (vapor or immersed), temperatures {90 and 60 °C [194 and 140 °F]}, and sample geometries (creviced and noncreviced samples) in the Long-Term Corrosion Test Facility were used as input data to computations in CRWMS M&O (2000b). The cumulative density function of the Alloy 22 experimental corrosion rates (2-year data) is displayed in Figure 3-7. The negative rates have been interpreted by DOE as caused by silica deposits on the experimental samples. For performance assessment computations, DOE ignored apparent negative rates and corrected the experimental distribution of corrosion rates by the addition of a uniform distribution ranging from 0 to 63 nm/yr [2.48×10^{-6} in/yr] (CRWMS M&O, 2000i). The resulting corrected cumulative distribution is displayed in Figure 3-7. The corrected distribution overlaps corrosion rate data for the file WDgA22SR00.cdf, which contains input corrosion rates for the median case run in the SR00_037ne6.gsm file. These corrosion rate data are also practically identical to data reported in Figure 3.4-13 of CRWMS M&O (2000b).

The Gauss-Variance Partitioning method was applied to the corrected distribution of corrosion rates, and results are presented in Figure 3-8. In Figure 3-8(a), it is noted that (i) each derived distribution (grey lines) contains the extreme corrosion rates in the limit when enough samples are gathered, and (ii) the original distribution of rates is reconstructed from the Gauss-Variance Partitioning distributions. Point (i) is important because the failure time of waste packages is controlled by the highest corrosion rate. Point (ii) is important because it shows that, on average, the Gauss-Variance Partitioning method preserves the frequency of the distribution of corrosion rates. For the median-case computations of the SR00_037ne6.gsm file, Alloy 22 corrosion rates were sampled from a Gauss-Variance Partitioning distribution with 50-percent variance, centered at the median corrosion rate. This distribution of rates is contained in the file WDdA22SR00.cdf. Both the original and the Gauss-Variance Partitioning distributions of corrosion rates are displayed in Figure 3-8(b). Data in the file WDdA22SR00.cdf compare well to the independent computations.

3.3.2.3.2.1 A Simplified Model for General Corrosion

In this section, a simplified algorithm is discussed to review general corrosion computations by the WAPDEG code. First, some important features and definitions of the WAPDEG code are discussed. In the WAPDEG code, the surfaces of the waste packages and drip shields are discretized into 1,000 patches and 500 patches, respectively. Four hundred waste package–drip shield pairs are simulated to derive confidence intervals. Presumably, this extent of discretization is enough to guarantee convergence of quantities such as the time of first patch failure and fraction of failed surface as a function of time (CRWMS M&O, 2000g). Within WAPDEG, a patch is considered failed if the corrosion front has completely penetrated the thickness of the waste package or drip shield.

Within WAPDEG, corrosion rates of the waste package are corrected to account for microbially influenced corrosion and thermal aging. Microbial induced corrosion is assumed to affect the

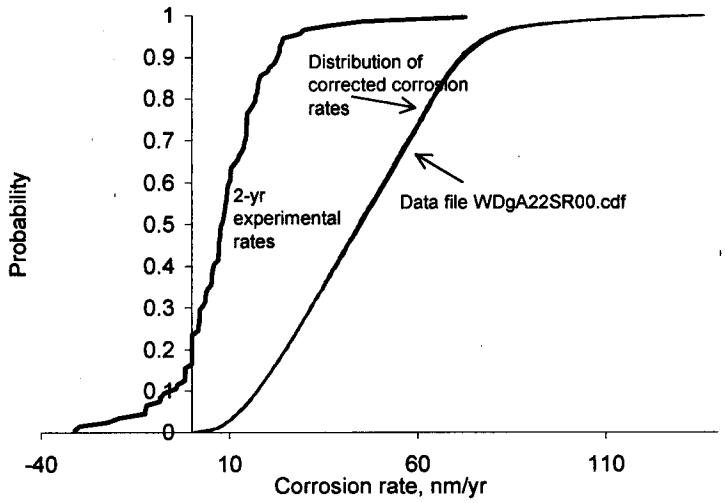

Figure 3-7. Cumulative Distribution Function of Corrosion Rates Measured in A 2-year Period in the Long-Term Corrosion Test Facility. The Two Overlapping Lines on the Right Side of the Figure Correspond to Data in the File WDgA22SR00.cdf and Data Derived by Ignoring Negative Corrosion Rates and Applying a Correction Sampled from a uniform distribution Ranging from 0 to 63 nm/yr [2.48×10^{-6} in/yr].

body of the waste package, and the action of microbially influenced corrosion is described by modifying the corrosion rates by an enhancement factor sampled from a uniform distribution ranging from 1 to 2. The microbially influenced corrosion factor is activated only after the relative humidity of the waste package environment has exceeded 90 percent. Thermal aging is assumed to affect only the closure weld area, and its action is presumably accounted for by enhancing corrosion rates by a factor uniformly distributed in the range 1 to 2.5. The thermal aging enhancement factor is assumed always present, however, it affects only a minor fraction of the total surface area of the waste package, namely the closure weld area. General corrosion starts in WAPDEG when the relative humidity around the waste package exceeds a deliquescence point value (of the order of 50 percent) that depends on the temperature. Below the deliquescence point, a dry environment is assumed and aqueous corrosion are not initiated. After any patch on the surface is penetrated, establishment of an aqueous environment inside the waste package is assumed and corrosion from the inside to the outside of the waste package is activated.

A simplified model was constructed to perform a review of the WAPDEG general corrosion model. In the simplified model, we assumed that general corrosion is activated at time = 0. This simplification neglects the delay in the establishment of aqueous corrosion. This delay is of the order of 500 years, which is not significant for waste packages that fail in the order of 100,000 years. It is also assumed that the microbially influenced corrosion factor is in effect at time = 0. The time needed for a 90-percent relative humidity to be established is of the order of 1,000 years. This time is also not significant for long-lasting waste packages. Our simplified computations provide a lower bound for the failure time. The more detailed computations from WAPDEG should yield failure times comparable to the simplified computations, plus 1,000 years at most.

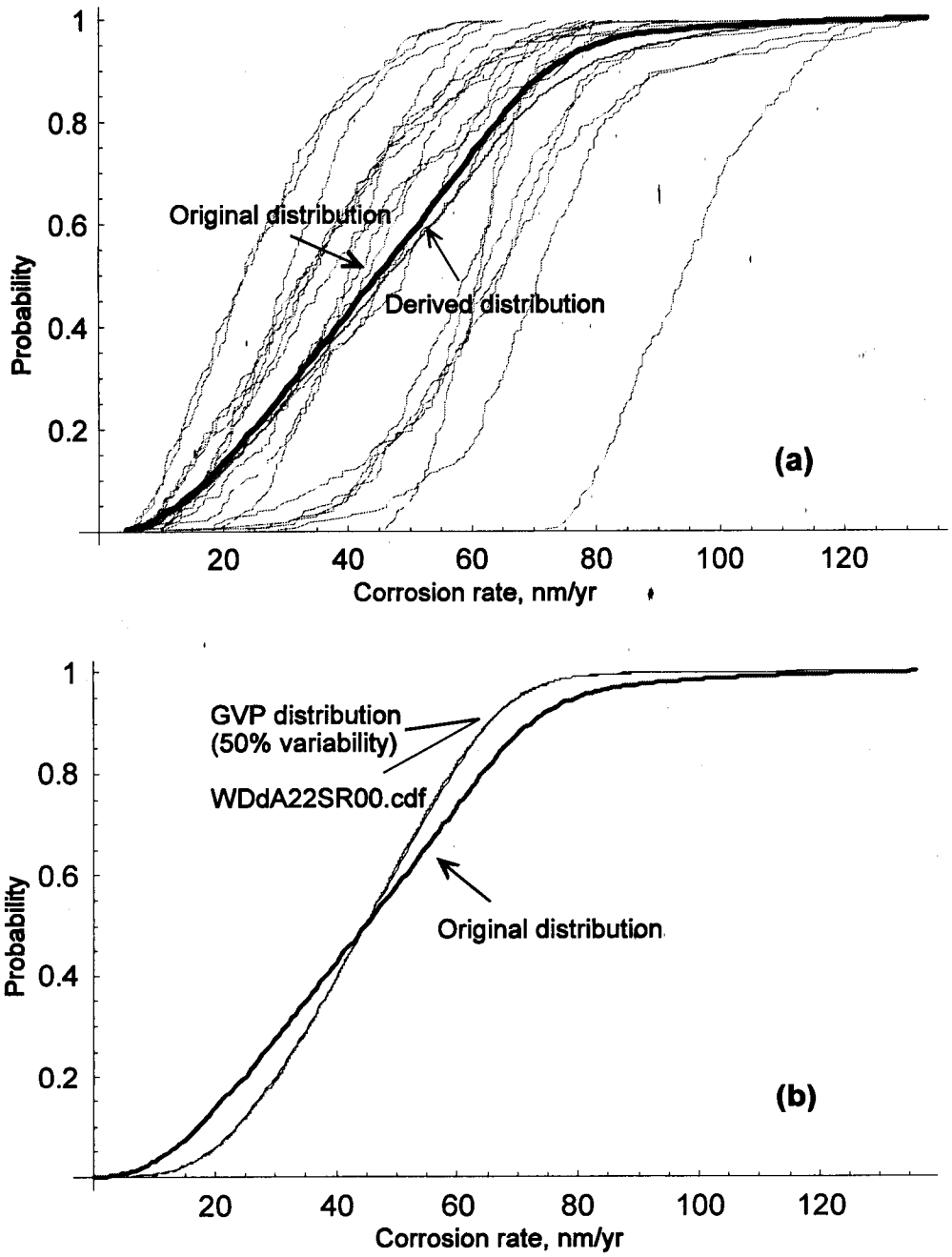

Figure 3-8. (a) Output of the Gauss-Variance Partitioning Method Applied to the Distribution of Corrosion Rates of Alloy 22, Sampling the Uncertainty Fraction Uniformly In the Range (0,1). The Thick Line Represents the Original Cumulative Distribution Function of Corrected Corrosion Rates of Alloy 22. The Background Grey Lines Are Distributions Derived by the Gauss-Variance Partitioning Method. The i. (b) The Gauss-Variance Partitioning Method Was Applied to the Distribution of Corrosion rates, Selecting a 50 Percent Variability and Centering the Variability Distribution at the Median Corrosion Rate. The Gauss-Variance Partitioning Distribution overlaps with the Distribution Defined in the File Wdda22sr00.cdf.

The Gauss-Variance Partitioning method was not used to produce subdistributions of corrosion rates from the original distribution of rates. The justification for this simplification is that the Gauss-Variance Partitioning method does not yield different information than that contained in the original distribution of rates. In particular, the derived subdistributions by the Gauss-Variance Partitioning method contain the end points of the original distribution in the limit when the population size tends to infinity. If the Gauss-Variance Partitioning method is used to sample corrosion rates, and the average failure time from a large number of subdistributions is computed, the average failure time should be equivalent to the one derived by considering only the original distribution of rates. Because the interest is only in average failure times (and not in defining confidence intervals for these average values), in the simplified model a unique distribution function for corrosion rates is used. Also, the use of only one distribution of rates facilitates inquiries on convergence issues.

3.3.2.3.2.2 First Patch Failure

This section describes the algorithm to determine the fraction of waste packages with at least one patch failed as a function of time (referred to as first patch failure curve or failure curve). The first patch failure is an important quantity because it determines the time for the activation of corrosion from the inside of the waste package to the outside. The first patch failure curve is frequently used by DOE to present results of sensitivity analysis as an intermediate measurement of repository performance. In this section, it is argued that the first patch failure curve converges to a step function in the limit when the waste package discretization tends to infinity (i.e., in the limit when a large number of patches is considered). The time at which the step is located is determined by the maximum corrosion rate. The algorithm to compute first patch failure is described next.

Step 1) Populate the waste package patches with rates sampled from the corrected distribution of corrected corrosion rates (see Figures 3-7 and 3-8).

Step 2) Apply a random factor to the sampled corrosion rates that is selected from a uniform distribution ranging from 1 to 2, to account for microbially influenced corrosion.

Step 3) Select at random the patches that represent the closure weld area (if the fraction of the surface covered by closure welds is 0.03, then 30 patches from 1,000 represent the closure weld area).

Step 4) For the closure weld patches, apply a random factor selected from a uniform distribution ranging from 1 to 2.5 (to account for thermal aging correction to the sampled corrosion rates).

Step 5) Compute failure times as time = thickness/rate, where the corrosion rate contains the appropriate corrections (microbially influenced corrosion and thermal aging corrections). The thickness of the waste package body is 2 cm [0.78 in], and the total effective thickness of the closure weld is 3.5 cm [1.38 in]. The closure weld is made of two components: a 2.5-cm [0.98-in] thick weld on the external lid, and a 1 cm [0.39 in] thick weld on the internal flat lid.

Step 6) Keep record of the minimum time. This is the first patch failure time.

Step 7) Repeat 1–6 a number of times (DOE uses 400 iterations = 400 waste packages in WAPDEG) to derive confidence intervals for the time to first patch failure.

The corrosion rates used in the computations were selected from the distribution defined in the file WDdA22SR00.cdf. The maximum corrosion rate therein reported is 136 nm/yr [5.4×10^{-10}].

It was considered that 3 percent of the patches are closure weld patches. This value was derived by inspecting the contents of the GoldSim variable, WP_Inner_Cracks, in the SR00_037ne6.gsm file. Therein, the maximum number of patches affected by crack failure is 29.772 from a total of 1,000. Because crack failure only affects the weld area, it follows that the considered weld area in the median value TSPA–GoldSim code run is approximately 3 percent of the total surface.

In the discussion that follows, a waste package is considered failed if the general corrosion front has penetrated at least one patch either from the body of the waste package or the weld surface. The dependence of the fraction of waste packages failed as a function of time on the number of patches is displayed in Figure 3-9.

The curve for the fraction of waste packages failed has not reached convergence after consideration of 10,000 patches on the waste package surface. The convergence function can be anticipated, however. The minimum possible failure time of the closure weld surface is

$$t = \frac{3.5 \times 10^7 \text{ nm}}{2 \times 2.5 \times 136 \text{ nm / yr}} = 51{,}471 \text{ yr} \qquad (3\text{-}13)$$

The minimum possible failure time of the body of the waste package is

$$t = \frac{2 \times 10^7 \text{ nm}}{2 \times 136 \text{ nm / yr}} = 73{,}529 \text{ yr} \qquad (3\text{-}14)$$

The number 2 in the denominator of Eqs. (3-13) and (3-14) is the maximum microbially influenced corrosion factor. The first patch failure curve of Figure 3-9 seems to be converging to a step function located at 73,529 years. As the number of patches increases, however, the population of patches on the weld area will be large enough to have a corrosion rate arbitrarily close to the extreme value of 2 × 2.5 × 136 nm/yr = 680 nm/yr [26.77 × 10^{-6} in/yr]. In the limit when the number of patches tends to infinity, all of the waste packages will have a corrosion rate arbitrarily close to the extreme value, and, therefore, all of the waste packages will fail at the same time (51,471 years). If more detailed computations accounting for the relative humidity changes were performed, the limit convergence curve would still be similar to a step function, which step is not sharply located at a single time, but would range from 51,000 to 53,000 years. After approximately 53,000 years, all waste packages should have at least one patch that has been penetrated by general corrosion on the closure weld area.

Figure 3-9 includes a comparison of the fraction of waste packages failed by general corrosion in the TSPA–GoldSim code median run to our independent computations. The TSPA–GoldSim code data are available in the variable named WPIB_1st_Patch of the file SR00_037ne6.gsm. A significant difference is noted. Because the WAPDEG is implemented as a dynamic link library external to TSPA–GoldSim code, it is not possible to track the source of the differences by browsing the SR00_037ne6.gsm file. Accounting for the variation in the relative humidity is not sufficient to explain the differences. It is suspected that the source of the difference is in the algorithm for the sampling of corrosion rates.

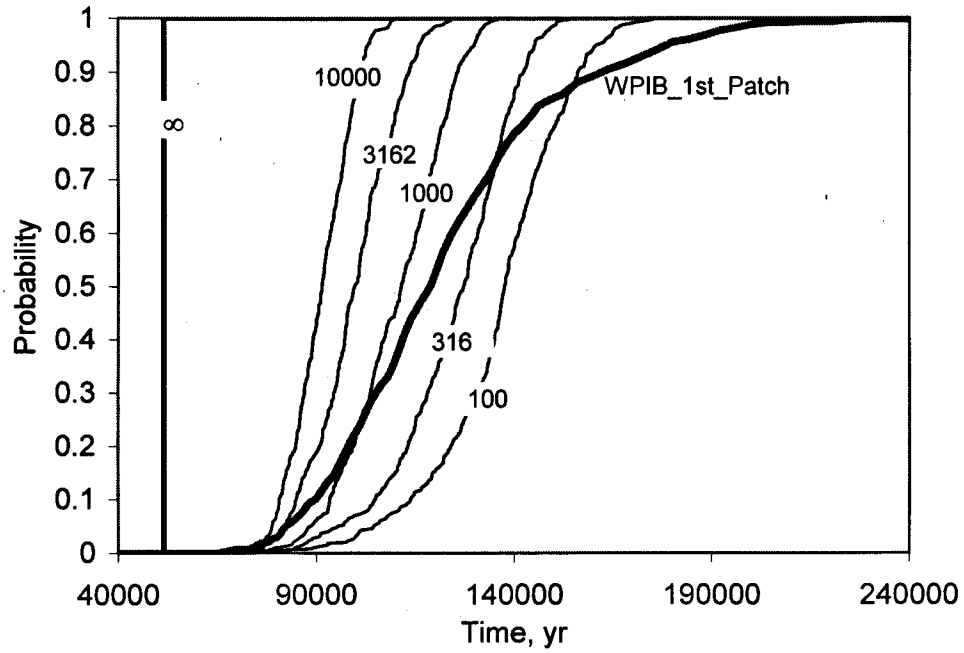

Figure 3-9. Fraction of Waste Packages with at Least One Patch Penetrated by General Corrosion as a Function of Time. The Numbers in the Figure next to the Lines Are the Number of Patches on a Waste Package Surface. The Thick Line Includes Data of the TSPA–GoldSim Code Median Run Contained in the Variable Named WPIB_1st_Patch.

We conclude that it is incorrect to use the first-patch failure curves (such as those shown in Figure 3-9) to measure the performance of the system for two reasons: (i) convergence is not achieved by consideration of 1,000 patches and (ii) the convergence function is solely dependent on the maximum corrosion rate. It has been argued elsewhere (CRWMS M&O, 2000g) that 1,000 patches are enough to guarantee convergence of the first-patch failure curve, but this conclusion is in contradiction with the simplified computations in this report. It must be noted, however, that infinite discretization of the waste package surface lacks physical meaning. Also, the variability in the corrosion rates measured in the Long-Term Corrosion Test Facility may be valid only for patches similar in area to the test samples. In other words, it may not be appropriate to assume the same distribution of corrosion rates on much smaller areas than those of the coupons of the weight-loss experiments. Within the TSPA–GoldSim code implementation further exploration is recommended of the factors determining the shape of the first-patch failure curve to sort this apparent convergence problem.

3.3.2.3.2.3 Fraction of Corroded Waste Package Surface as a Function of Time

After the general corrosion front has penetrated any patch, it is assumed an aqueous or humid environment is established inside the waste package. Clearly this assumption is not valid if the patch is infinitely small; therefore, a limit should be established on the maximum meaningful

discretization of the waste package surface. Assuming that t_{min} is the time of the first-patch penetration, the penetration time for any patch is computed in the simplified approach as

$$t = t_{min} + \frac{d - r \times t_{min}}{2 \times r} \quad (3\text{-}15)$$

where d is the initial thickness {2 cm [0.78 in] for the body of the waste package or 3.5 cm [1.38 in]} for the closure weld area) and r is the corrosion rate for a particular patch. After the first patch penetration time, t_{min}, it is assumed that r is the corrosion rate for both the exterior and interior patch surfaces. Thus, the total effective corrosion rate after t_{min} is $2 \times r$, and the time needed for the corrosion fronts (outside-inside and inside-outside) to dissolve the remaining thickness, $d - r \times t_{min}$, equals $(d - r \times t_{min})/(2 \times r)$. Note that in WAPDEG the inside-outside rate is sampled independently from the outside-inside rate. This different sampling approach should not yield a major divergence between the simplified analysis and the WAPDEG computations. As last step in the simplified computations the collection of penetration times for each patch is tracked, and the cumulative distribution function for the population of failure times is computed. This cumulative distribution function can be interpreted as the fraction of patches penetrated by general corrosion as a function of time. Two approaches were followed to define t_{min}. In the first approach, t_{min} was defined as the time of first-patch penetration (Subsection 3.3.2.3.2.2). In the second approach, t_{min} = 51,471 years. This latter approach yields the convergence curve in the limit when the number of patches is very large. The results from the computations are presented in Figure 3-10.

In Figure 3-10, important differences are noted between the limiting curve for the fraction of failed patches versus time and those curves derived when 1,000 or 10,000 patches are considered. The difference is significant, especially in the first 100,000-year period [Figure 3-10(b)]. There is good agreement between data contained in the variable WP_Inner_PatchFailures of the TSPA–GoldSim code median run and the simplified computations in the 100,000-year period. Significant disagreement is noted for longer periods, however. Differences in the sampling strategy (e.g., selection of the inside-outside corrosion rate independently from the outside-inside rate and modeling of the waste package Alloy 22 wall as composed of two virtual independent layers) are not envisioned enough to account for the disagreement. It is possible, however, the collection of corrosion rates used as the starting point in the simplified computations (those defined in the file WDdA22SR00.cdf; see Figure 3-8) may differ from the rates actually used in the TSPA–GoldSim code median run.

We concluded that the use of 1,000 patches may not be enough to guarantee convergence of the curve for the fraction of patches failed versus time. As previously mentioned, however, care must be applied to use a distribution of corrosion rates to infinitely small patches because (i) the experimental distribution of corrosion rates has associated an intrinsic scale fixed by the area of the coupon samples of the weight-loss experiments, and (ii) certain model-hypotheses cease to be valid (e.g., the activation of inside-outside corrosion after first-patch penetration). Although the convergence argument for the selection of 1,000 patches offered in CRWMS M&O (2000g) may not be valid, the discretization into 1,000 patches may be justifiable on the basis of the size of the weight-loss coupons used to derive a distribution of corrosion rates.

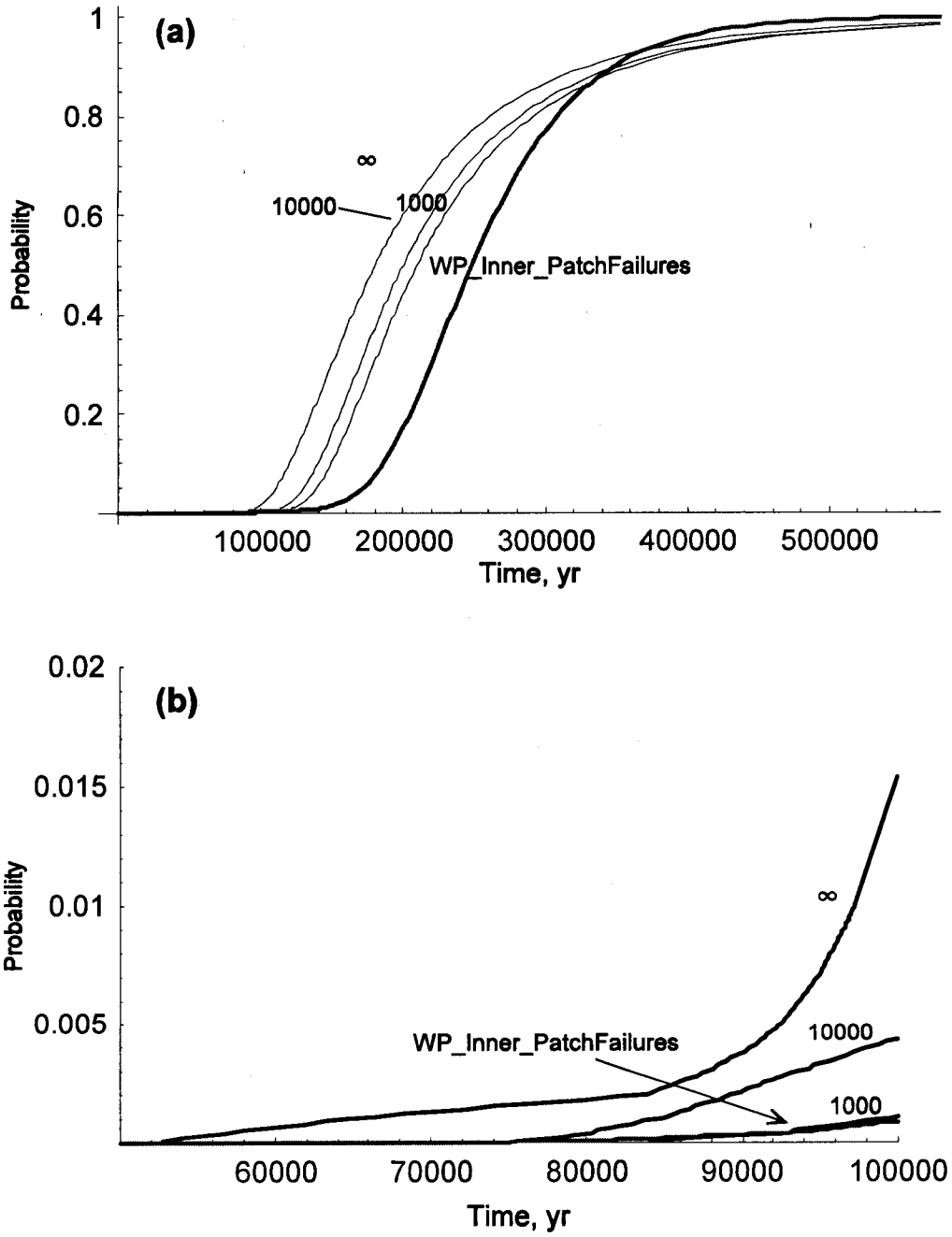

Figure 3-10. Fraction of Patches Penetrated by General Corrosion as a Function of Time. (a) and (b) Are the Same Plots in Two Different Time Ranges. The Numbers 1,000 and 10,000 Represent the Number of Patches Considered in Generating the Figures. The Symbol ∞ Labels the Convergence Cumulative Distribution in the Limit When a Large Number of Patches Is Considered. Data from the SR00_037ne6.gsm File Contained in the Variable Named WP_Inner_PatchFailures Are Also Included.

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A second conclusion of the simplified analysis is, provided that the appropriate collection of corrosion rates was used, the divergence between data in the TSPA–GoldSim variables (WP_Inner_PatchFailures and WPIB_1st_Patch) and our computations can be explained only from features of the WAPDEG currently not understood. If characteristics such as the time needed to establish a relative humidity above deliquescence (to initiate general corrosion, presuming localized corrosion does not occur) and above 90 percent (to activate the microbially induced corrosion enhancement factor) and the possible dependence of the corrosion rate on the temperature are features that are ignored, the WAPDEG algorithm can be simplified to compute the first-patch failure time and the fraction of patches failed. Results from simplified computations should be in close agreement from those derived from the detailed WAPDEG algorithm. Simplified computations could be used as verification tools of model implementation. We verified that the correction to corrosion rates to account for silica deposits is in agreement with DOE documentation and that the Gauss-Variance Partitioning method is well implemented within WAPDEG. That the computations to determine waste package failure and the extent of the failure by general corrosion are in agreement with DOE documentation has not, however, been verified.

3.3.2.3.2.4 Modification to Seepage Rate by Waste Package and Drip Shield Failure

This section discusses how information, such as the fraction of patches failed as a function of time, is used in downstream modules of the TSPA–GoldSim code. The extent of the degradation of the waste package and drip shield surfaces is used to estimate the amount of water available for advective release. According to descriptions in CRWMS M&O (2000b,h), the extent of the corroded surface is projected along the axial direction of both the waste package and the drip shield, and the fractional length is used as a modulating factor to the amount of seepage at the drift. The resulting product is an estimate of the amount of water available for radionuclide release. Figure 3-11 can facilitate understanding of the concept of fraction of degraded axial length. In the figure, the fraction of failed patches is 5/24. To compute the fraction of degraded axial length, the number of circumferential strips containing at least one black patch must be counted. There are 6 circumferential strips, and 3 contain at least 1 black patch; thus, the fraction of degraded axial length is 3/6 = 0.5.

It is argued in CRWMS M&O (2000b,h) that the use of the fraction of degraded axial length as a factor to determine the amount of water available for release computations is a conservative approach. It is assumed that water dripping on any part of the waste package surface could slide along the circumferential direction and be captured by any failed patch on the circumference path. This assumption is clearly conservative because it disregards the fact that water cannot move upward against gravity. In reality, capture of the drip is only possible by failed patches located not only on the circumferential path but below and on the same side of the drip position.

The fraction of degraded axial length and the fraction of failed patches are correlated quantities (but are not linearly related). It is a combinatorial problem to derive the most likely degraded axial length fraction for a particular value of the fraction of failed patches. The solution to this problem cannot be derived analytically, but it is intuitive that the fraction of degraded axial length depends on the number of patches. In the limit when the number of patches tends to infinity, the population of patches located along any circumferential strip (*C* direction in

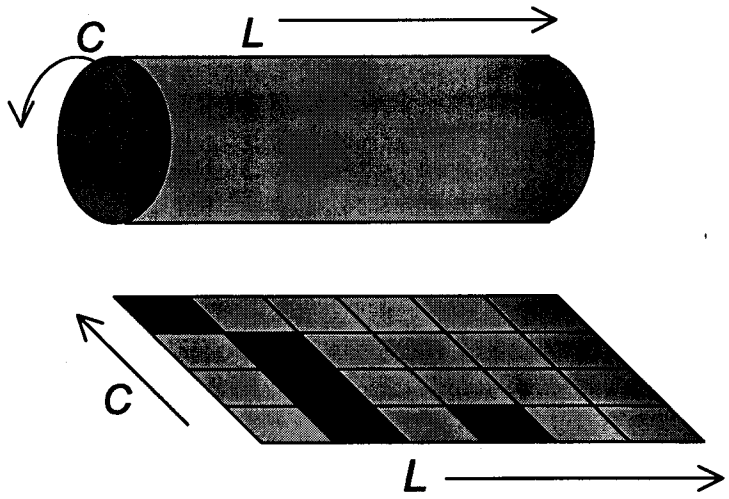


Figure 3-11. Flattened Waste Package Surface. L Is the Axial Direction and C Is the Circumferential Direction. The Black Patches Represent Failed Patches. In this Example, the Fraction of Failed Patches is 5/24, and the Fraction of Degraded Axial Length Is 3/6 = 0.5.

Figure 3-11) will be large enough to include a patch with a corrosion rate arbitrarily close to the maximum corrosion rate {(2 × 136 = 272 nm/yr [10.71 × 10^{-6} in/yr]}. Thus, in the limit when the number of patches tends to infinity, all circumferential strips contain a patch failing at 73529 year. Thus, the fraction of degraded axial length versus time converges to a step function, with step located at 73,529 years. The concept of fraction of degraded axial length can be mathematically extended to include the lids and the weld closure area of the waste package; the main ideas to do so were developed in CRWMS M&O (2000h). It is noted that the fraction of degraded axial length depends on the discretization, and, in the limit when the number of patches tends to infinity, the fraction of degraded axial length converges to a two-step function (one step located at 51,471 year and a second at 73,529 year).

The TSPA–GoldSim code implementation is not in agreement with DOE documentation. The fraction of degraded axial length within TSPA–GoldSim is incorrectly computed. TSPA–GoldSim code defines the fraction of degraded axial length to be linearly proportional to the number of patches failed on the waste package surface. More specifically, the fraction of degraded axial length is computed as (number of patches failed) × (patch length)/(waste package axial length). This definition was determined by inspecting the GoldSim variable WP_Frac_Patch_CSNF (a similar definition is employed for codisposal waste packages). Also, the presumed fraction does not range between zero and one, but can exceed one. To correct that problem, the quantity WP_Frac_Patch_CSNF is artificially truncated at one within TSPA–GoldSim code, before using it as a factor to estimate the amount of water available for advective release. The definition of WP_Frac_Patch_CSNF in the TSPA–GoldSim code lacks physical meaning, and it is inconsistent with the DOE documentation.

For the drip shield, the DOE documentation states that the fraction of degraded axial length of drip shield is used to modulate the amount of water available for release (CRWMS M&O,

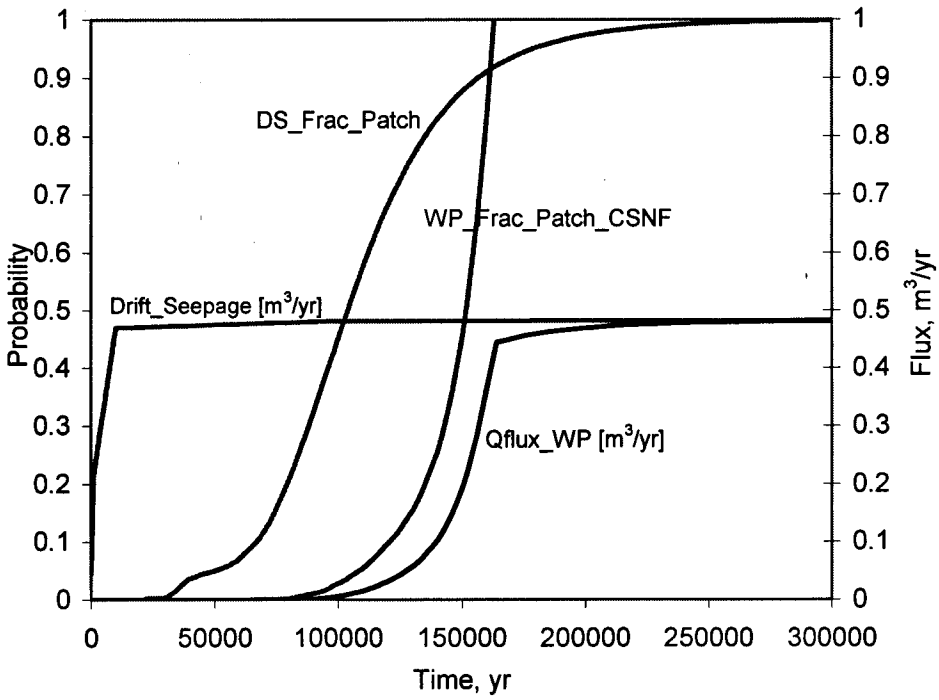
2000b). In TSPA–GoldSim code, however, the fraction of failed patches is directly used to modulate the amount of water. This is evident from the definition of the variable Qflux_DS=Drift_Seepage × DS_Frac_Patch (DS_Frac_Patch is the fraction of patches failed as a function of time).

Figure 3-12 is provided to assess the significance of the noted inconsistency in TSPA–GoldSim code. Figure 3-12(a) presents the derivation of the amount of water for the computation of advective release within the TSPA–GoldSim code and the data for the median case run (SR00_037ne6.gsm file). The variable Drift_Seepage tracks the amount of seepage at the drift in m^3/yr units. This seepage rate is modulated by the fraction of patches failed on a drip shield, DS_Frac_Patch, and the axial degraded length of a waste package, WP_Frac_Patch_CSNF. The resulting water flux, Qflux_WP=Drift_Seepage × DS_Fract_Patch × WP_Frac_Patch_CSNF, is the amount of water available for the advective release of radionuclides. Figure 3-12(b) includes fluxes that would be derived if more consistent definitions were applied. For example, the dotted line (1) would be obtained if the approach explained in CRWMS M&O (2000h) were indeed implemented to determine the amount of water available for advective release. The dotted line (2) would be obtained if the fraction of patches failed, for both the drip shield and the waste package, was used as a factor to modulate the seepage rate at the drift. Clearly, the current implementation in the TSPA–GoldSim code is conservative with respect to option (2). The current implementation however, is not conservative with respect to the proposed approach in the DOE documentation. Besides, the variable WP_Frac_Patch_CSNF lacks physical meaning, as previously explained.

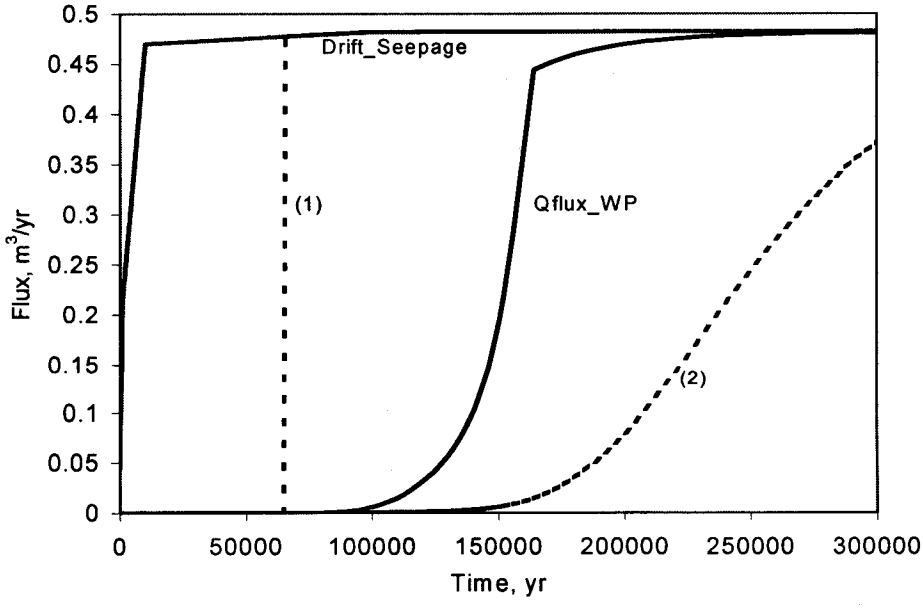
3.3.2.3.3 Stress Corrosion Cracking

Stress corrosion cracking is assumed to affect only the closure weld area of the waste package, and not the drip shield. The stress corrosion cracking model used in the nominal scenario of the DOE total system performance assessment model is known as the slip-dissolution model. In this model, it is assumed that cracks oriented radially on the closure weld area can grow due to hoop stress, provided the conditions leading to stress corrosion cracking are met. In the slip-dissolution model, crack propagation occurs when the stress intensity factor is in excess of a threshold value determined by a normal distribution centered around 33 MPa $m^{1/2}$ [30 ksi $in^{1/2}$] (CRWMS M&O, 2000j). The stress intensity factor is negative at the surface of the closure welds of the outer and inner lids, because processes (induction-heating solution annealing in the outer closure-lid welds and laser peening in the inner closure-lid welds) will be used to relieve tensile stresses. The stress intensity factor is positive at a distance on the order of 1 cm [0.39 in] for the closure weld on the outer lid and 0.5 cm [0.2 in] for the weld on the inner lid (CRWMS M&O, 2000j, Figures 4 and 8).

The propagation velocity of the tip of the crack is computed by a power law on the stress intensity factor. The coefficient and the exponent of the power law are uncertain and sampled from distribution functions. In the case of stress corrosion cracking activation, failure occurs in a relatively short time (CRWMS M&O, 2000j). Information, such as incipient crack density and size and preexisting manufacturing defects in the closure-lid welds, apparently also is used by the slip-dissolution model (CRWMS M&O, 2000j; Lee et al., 2002). The dimension of the cracked area as a function of time is used as input to diffusive release computations in the TSPA–GoldSim code model.



(a)



(b)

Figure 3-12. (a) The TSPA–GoldSim Code Derivation of the Flux of Water Available for Advective Release: Qflux_WP = Drift_Seepage × DS_Fract_Patch × WP_Frac_Patch_CSNF. (b) The Dotted Line as (1) Would Be Obtained If the Approach Explained in CRWMS M&O (2000h) Was Implemented to Determine the Amount of Water Available for Advective Release. The Dotted Line (2) Would Be Derived If the Fraction of Patches That Failed for the Drip Shield and the Waste Package Was Used to Modulate the seepage Rate at the Drift.

Documentation on the implementation describing the stress corrosion cracking model was reviewed and not enough information was found for particular aspects. For example, it is unclear how the number of cracks on the closure-lid weld is computed in the implementation of the slip-dissolution model within WAPDEG, and also how the number of defects from the manufacturing defect abstraction model is used in the slip-dissolution model. It appears the defect size computed from the manufacturing defect abstraction model is compared to an incipient size, and if the defect size exceeds the incipient size, the defect is a potential site for stress corrosion cracking. However, the connection, between the number of defects derived from the manufacturing defect abstraction model and the number of cracks from the slip-dissolution model is uncertain. There is no summary of the implementation of this aspect within WAPDEG in the DOE documentation.

The number of closure-weld patches affected by stress corrosion cracking is tracked by WAPDEG and the TSPA–GoldSim code. The GoldSim variable WP_Inner_Cracks tracks the number of closure-weld patches failed by stress corrosion cracking as a function of time. The area of the surface affected by stress corrosion cracking, WP_Total_Crack_Area, is computed as WP_Total_Crack_Area = WP_Inner_Cracks × WP_Crack_Area × Cracks_per_Patch_Factor. WP_Crack_Area is a constant equal to the cross section of a single crack: 4.08×10^{-6} m^2 [6.32×10^{-3} in^2] (CRWMS M&O, 2000h). Cracks_per_Patch_Factor is the assumed number of cracks on a patch of the closure-weld area. No reference was found to this variable in the DOE documentation. The value of Cracks_per_Patch_Factor in the SR00_037ne6.gsm file is 10. On page 79 of CRWMS M&O, (2000i), it is stated that approximately one radial crack per closure weld patch was considered in the total system performance assessment; this DOE document refers to Section 5 of CRWMS M&O (2000j) to justify this selection. Section 5 of CRWMS M&O (2000j) was reviewed, and there is no information on the number of radial cracks per closure-weld patch. It seems the computed number of cracks by the slip-dissolution model of WAPDEG is much greater than the number of manufacturing defects (few packages are affected by closure-weld defects—one or two at most on each waste package). The outcome of the slip-dissolution model, within WAPDEG, appears independent of the computed number of manufacturing defects.

It is clearly evident that the number of cracks on a waste package computed by GoldSim depends strongly on the parameter Cracks_per_Patch_Factor and also on the number of patches. Increasing the number of patches causes an increase in the quantity WP_Total_Crack_Area. Furthermore, the definitions in the TSPA–GoldSim code do not seem to preclude the case WP_Total_Crack_Area > closure-weld area, which does not make physical sense. There are no sensitivity studies in CRWMS M&O (2000g) on the effect of the number of patches on the size of the area affected by stress corrosion cracking. Those analyses should reveal the predicted dependence. Selecting the appropriate dimensions of the stress corrosion cracking area is important because importance and sensitivity analyses in CRWMS M&O (2000b) convey relevance to stress corrosion cracking.

A possibility to verify the consistency of the WAPDEG implementation of the slip-dissolution model with the DOE documentation is to perform simplified computations. Simplified computations were not completed because of the limited scope of this review and also because the divergence in the general corrosion model should be sorted first. Possible simplifications to perform a review of model implementation are outlined next. The propagation velocity of the tip of the crack could be ignored. For example, it could be assumed that the tip of the crack penetrates the weld thickness instantaneously if stress corrosion cracking is

activated. The time of failure would be determined by the time for the general corrosion front to penetrate the thickness of the compressive stress region (defined as the region with stress intensity factor less than the threshold stress intensity factor for stress corrosion cracking). This thickness varies as a function of the uncertainties in the stress intensity factor and the threshold stress intensity factor. It may be possible to directly derive a distribution for the thickness of the compressive stress region. Thus, failure times by stress corrosion cracking could be computed by directly sampling thicknesses and corrosion rates. The failure time for a particular patch can be approximated as the ratio of the compressive stress region thickness and the corrosion rate. This proposed simple approach could provide a verification of the implementation of the complex stress corrosion cracking algorithm in WAPDEG and also yield relevant information on the important elements of the model. It is anticipated that the results of the stress corrosion cracking model are a strong function of the distribution of general corrosion rates and the maximum general corrosion rate. This functionality may not be revealed by conventional sensitivity and uncertainty analyses, because this maximum corrosion rate is usually not varied.

3.3.3 Summary

Explicit documentation on the parameter Cracks_per_Patch_Factor was not found. This parameter of the TSPA–GoldSim code model is important because it is used to compute the size of the closure-weld area affected by stress corrosion cracking. Also, not enough information was found on the vector WAPDEG_inputs. This vector contains more that 1,000 entries, without units or comments. Without documentation, the adequacy of the information contained therein cannot be established.

An analysis of the implementation of the Gauss-Variance Partitioning method, general corrosion, and stress corrosion cracking within WAPDEG was presented. It was concluded that the Gauss-Variance Partitioning method preserves the information of the distribution of corrosion rates, and each Gauss-Variance Partitioning distribution contains the extremes of the original distribution. Results from our independent analyses are consistent with the DOE results, and the Gauss-Variance Partitioning method seems well implemented within WAPDEG and theTSPA–GoldSim code.

For general corrosion, the distribution of corrosion rates for total system performance analyses from the collection of experimental corrosion rates and guidelines in the DOE documentation was reproduced. The WAPDEG model, however, could not be verified, because there was significant disagreement between simplified computations and the results in the SR00_037ne6.gsm file.

It was argued that the fraction of waste packages with at least one patch penetrated by general corrosion as a function of time depends on the number of patches on the waste package surface. Therefore, this quantity may not be an appropriate secondary measurement of repository performance. It was also argued that the fraction of patches failed on a waste package surface as a function of time requires more than 10,000 patches to achieve convergence. It was noted, however, that use of infinitely small patches may not be a valid approach because (i) the variance of the corrosion rates may be valid only for a particular patch surface size, and (ii) model assumptions break for extremely small patches

(e.g., the assumption of activation of corrosion from the inside of the waste package to the outside after first-patch breaching).

An inconsistent definition was noted for the fraction of degraded axial length for the waste package. This quantity is used as a factor to modify the seepage rate at the drift to estimate the amount of water available for radionuclide release. The definition implemented in the the TSPA–GoldSim code lacks physical meaning and is not consistent with the DOE documentation. The DOE documentation (e.g, CRWMS M&O, 2000b) states that the fraction of degraded axial length for the drip shield is used as a factor to modulate the seepage rate at the drift. The modulating factor used in TSPA–GoldSim code, however, is the fraction of patches failed by general corrosion as a function of time. Figure 3-12 presents an assessment of the effect of the noted inconsistencies on the amount of water available for radionuclide release. It was noted that the approach described in the DOE documentation is conservative with respect to the approach implemented in the TSPA–GoldSim code.

There is no clear description in the DOE documentation on the relationship between the number of defects from the manufacturing defect abstraction model and the number of cracks from the slip-dissolution model. The latter seems independent or quasi-independent on the former. Also, there is no documentation on the effect of the number of patches on the size of the area affected by stress corrosion cracking. A strong dependence is predicted among these two items. Finally, some simplifications were proposed to the slip-dissolution model that could be used to support verification of model implementation within WAPDEG.

3.4 Colloid Release and Transport in the Engineered Barrier Subsystem

3.4.1 Model Input

The reviewed expressions, data, stochastic data, selectors, and one-dimensional table of the TSPA–GoldSim code pertinent to colloid release and transport models for the engineered barrier subsystem are shown in Table 3-4 and are discussed separately. Some of the parameters appeared in the TSPA–GoldSim SR00_037ne6.gsm file in multiple locations with different values. The footnote indicators in the table identify which particular instance of the parameter was reviewed. Table 3-4 shows the references against which the model element was checked, typically CRWMS M&O (2000c) and two analysis and model reports (CRWMS M&O, 2000k,l).

3.4.1.1 Expressions

For all but one expression, no deviations that would affect calculation results were found relative to their representation in the relevant analyses and model report in CRWMS M&O (2000c). [Expressions related to the invert in the engineered barrier subsystem were checked by analogy to the respective waste package expressions because the invert expressions were not discussed in detail in CRWMS M&O (2000c)]. Some expressions were simple transformations or TSPA–GoldSim code implementation tools that did not need to be compared to process model abstraction documentation in analyses and model reports.

Table 3-4. Reviewed TSPA–GoldSim Code Elements Related to Colloid Release and Transport	
Element	**References**
Expression	
Condition_D_Invert *	CRWMS M&O, 2000c,k
Condition_D_WP *	CRWMS M&O, 2000c,l
M_Col_Gw_B_Invert *	CRWMS M&O, 2000c,k
M_Col_Gw_B_WP *	CRWMS M&O, 2000c,l
CPu_Col_Wf_Irrev_Invert_b *	CRWMS M&O, 2000c,k
Solubility_Irrev_Colloid_Invert *	CRWMS M&O, 2000c
CPu_Col_Wf_Irrev_Pu239 *	CRWMS M&O, 2000c
CPu_Col_Wf_Irrev_Pu240 *	CRWMS M&O, 2000c
Solubility_IrrevColloids *	CRWMS M&O, 2000c
Mass_Pu239_Irrev *	CRWMS M&O, 2000c
condition_A_invert **	CRWMS M&O, 2000c,k
condition_B_invert **	CRWMS M&O, 2000c,k
condition_C_invert **	CRWMS M&O, 2000c,k
condition_D_invert **	CRWMS M&O, 2000c,k
condition_E_invert **	CRWMS M&O, 2000c,k
Data	**References**
I_hi_thresh_col	CRWMS M&O, 2000c,l
I_lo_thresh_col	CRWMS M&O, 2000c,l
M_Col_Feox_max	CRWMS M&O, 2000c,l
M_Col_Feox_min	CRWMS M&O, 2000c,l
CPu_Col_Wf_Irrev_min	CRWMS M&O, 2000c,l
CPu_Col_Wf_Irrev_max	CRWMS M&O, 2000c,l
Stochastic	**References**
Kd_wf_coll_Pu	CRWMS M&O, 2000c,l
Kd_wf_coll_Am	CRWMS M&O, 2000c,l
Kd_fe_coll_Pu	CRWMS M&O, 2000c,l
Kd_gw_coll_Pu	CRWMS M&O, 2000c,l
Kd_fe_coll_Am	CRWMS M&O, 2000c,l
Kd_gw_coll_Am	CRWMS M&O, 2000c,l

Table 3-4. Reviewed TSPA–GoldSim Elements Related to Colloid Release and Transport (continued)	
Element	**References**
Selector	
pH_invert_bound	CRWMS M&O, 2000c,m
pH_drip_case2	CRWMS M&O, 2000c,m
M_Col_FeOx_Invert *	CRWMS M&O, 2000c,k
M_Col_FeOx_WP *	CRWMS M&O, 2000c,l
M_Col_Gw_Invert_a *	CRWMS M&O, 2000c,k
M_Col_Gw_Invert *	CRWMS M&O, 2000c,k
M_Col_Gw_WP_a *	CRWMS M&O, 2000c,l
M_Col_Gw_WP *	CRWMS M&O, 2000c,l
CPu_Col_wf_Irrev_Invert *	CRWMS M&O, 2000c,k
CPu_Col_wf_Irrev_a *	CRWMS M&O, 2000c,l
Ionic_Str_Invert *	CRWMS M&O, 2000c,k,m
pH_Invert *	CRWMS M&O, 2000c,k
pH_drip_case3	CRWMS M&O, 2000c,m
1-D Table	**References**
KC_PU_GW_COLLOID	CRWMS M&O, 2000c
KC_AM_GW_COLLOID	CRWMS M&O, 2000c,m
* Evaluated only in CDSP_Packages\Infiltration_Bin_3\Intermittent_Drip † Evaluated only in CSNF_Packages\Infiltration_Bin_3\Intermittent_Drip	

An error was found in reviewing the expression Mass_Pu239_Irrev in the file SR00_037ne6.gsm, which is used for comparing the released colloidal Pu-239 to that available in the waste form. The second expression in Mass_Pu239_Irrev,

> (CPu_Col_Wf_Irrev_Pu239/M_Col_Wf_Both_WP_Irrev)* Colloid_MassFlux* MasterClock.Timestep_Length

is taken from Eq. (6-8) in CRWMS M&O (2000c). The transfer of Eq. (6-8) to the TSPA–GoldSim code is correct. The four terms in the equation were checked in the TSPA–GoldSim code and were found to be consistent with abstraction and implementation descriptions in CRWMS M&O (2000c,l). There was a mismatch of units, however. In the TSPA–GoldSim code, , the term CPu_Col_Wf_Irrev_Pu239 is defined in units of g/L , M_Col_Wf_Both_WP_Irrev in mg/L, Colloid_Mass_Flux in g/yr, and MasterClock.Timestep_Length in years. The first two terms, therefore, yield grams of colloidal Pu-239 per milligram of waste form colloid, while the third and fourth yield grams of waste form

colloid. The entire expression, therefore, without a unit correction for colloid mass would give an incorrect colloidal Pu-239 mass.

Expression condition_B_invert (Table 3-4) was found to represent correctly the abstraction described in CRWMS M&O (2000c,k), however, the abstraction itself was found to be in error. This error is discussed in Subsection 3.4.2.3.1.

3.4.1.2 Data

All the reviewed data elements (Table 3-4) were derived ultimately from the waste form colloid release analyses and model report (CRWMS M&O, 2000l). For all but one data element, the TSPA–GoldSim code values are consistent with that analyses and model report and with CRWMS M&O (2000c). The value for CPu_Col_Wf_Irrev_max refers to the maximum released plutonium concentration on waste-form colloids; the value listed in the analyses and model report as 8×10^{-8} mol/L [3×10^{-7} mol/gal], but as 6×10^{-8} mol/L [2.3×10^{-7} mol/gal] in the TSPA–GoldSim code and in CRWMS M&O (2000c). In CRWMS M&O (2000l), the laboratory data supporting the higher value in the analysis and model report are plotted in Figure 7, while the abstraction is shown in Figure 13. The laboratory results support the higher maximum concentration, i.e., 8×10^{-8} mol/L [3×10^{-7} mol/gal]. Although data elements M_Col_Feox_max and M_Col_Feox_min were deployed correctly in the TSPA–GoldSim code, the document (CRWMS M&O, 2000l) does not provide a technical basis for the assertion that these concentrations are each based on a reasonable conservative estimate (CRWMS M&O, 2000l).

3.4.1.3 Stochastic

All six reviewed stochastic elements are sorption coefficients for plutonium and americium onto colloids (Table 3-4). The plutonium distributions (Kd_wf_coll_Pu, Kd_gw_coll_Pu, and Kd_fe_coll_Pu) are correctly transferred from the relevant analyses and model report (CRWMS M&O, 2000l) to CRWMS M&O (2000c). The distributions for the americium values (Kd_wf_coll_Am, Kd_gw_coll_Am, and Kd_fe_coll_Am), however, are represented in the TSPA–GoldSim code as truncated lognormal rather than simply lognormal as in the analysis and model report. A technical basis is lacking for this change.

The source for these six distributions is cited in CRWMS M&O (2000l) as the Unsaturated Zone and Saturated Zone Transport Properties analyses and model report (CRWMS M&O, 2000o). This document did not report the supporting data in detail, however. Mean sorption coefficients for americium on silica, hematite, and montmorillonite were mentioned, but how these data were used to derive the model distributions was not discussed. The report also discussed kinetic effects that argue against the use of an equilibrium sorption assumption (CRWMS M&O, 2000o). It is beyond the scope of the present review to probe more deeply into the supporting data, but the development of these distributions is not transparent nor easily traceable.

3.4.1.4 Selector

Unless discussed in the following subsections, the reviewed selectors were found to implement correctly the abstractions discussed in the reports cited in Table 3-4.

3.4.1.4.1 pH_invert_bound

This selector defines the pH for the case in which relative humidity is less than 50 percent (CRWMS M&O, 2000c, p. 185). Based on the source for in-drift pH model data (CRWMS M&O, 2000m), the following are the appropriate pH values:

- 9.40 for 50–1,000 years (Period 2)
- 7.64 for 1,000–2,000 years (Period 3)
- 7.02 for 2,000–100,000 years (Period 4)

In addition, conditions for times after 100,000 years are assumed to be the same as for those in the 1,000–2,000-year period (CRWMS M&O, 2000c, p. 53). In both the TSPA–GoldSim code and CRWMS M&O (2000c), the following names are given to these values:

- pH_bound_a = 9.4
- pH_bound_b = 7.64
- pH_bound_c = 7.02.

Therefore, the modeled bounding pH value should be equal to pH_bound_a for up to 1,000 years, pH_bound_b for 1,000–2,000 years, pH_bound_c for 2,000–100,000 years, and pH_bound_b for later than 100,000 years. However, the pH_invert_bound selector in the TSPA–GoldSim code reads:

if	ETime<=1000{yr}	then	pH_bound_a
else if	ETime>1000{yr} and ETime<=2000{yr}	then	pH_bound_c
else if	ETime>2000{yr} and ETime<=100000{yr}	then	pH_bound_b
		else	pH_bound_b

The parameters in the right-hand column should be, from top to bottom, pH_bound_a, pH_bound_b, pH_bound_c, and pH_bound_b. In conclusion, the TSPA–GoldSim code implementation is incorrect, giving the wrong bounding pH for times between 1,000 and 100,000 years. Note that the discussion on p. 189 of CRWMS M&O (2000c) is also in error in that it indicates pH_bound_c for times after 100,000 years.

3.4.1.4.2 pH_drip_case2

This selector defines the in-drift pH for relative humidities between 50 and 85 percent. The TSPA–GoldSim code implementation is consistent with the model and data references (Table 3-4), but the time periods for pH_drip case2 are 50 years earlier (i.e., less than 950 years, 950–1,950 years, and 1,950 to 99,950 years). The purpose of this model manipulation is not clear and should be justified.

3.4.1.4.3 Ionic_Str_Invert

The selector Ionic_Str_Invert, which assigns the invert ionic strength value based on relative humidity, is implemented consistently with CRWMS M&O (2000c). Ionic strength is assigned either the bounding value defined by the selector Ionic_Str_Invert_Bound or is calculated using

one of two other selectors: I_drip_case2 or I_drip_case3. These other three selectors were also inspected and were found to point, as a function of time period, to values or look-up tables in a manner consistent with CRWMS M&O (2000c) and with values correctly transferred from a precipitates/salts calculation report (CRWMS M&O, 2000m). A few minor errors that would have little or no effect on the TSPA–GoldSim code calculations were found. First, the description of Ionic_Str_Invert_Bound on p. 189 of CRWMS M&O (2000c) incorrectly assigns I_bound_c to times after 100,000 years; despite this, the TSPA–GoldSim code correctly uses I_bound_b. Second, the descriptions of I_bound_a, I_bound_b, and I_bound_c in the TSPA–GoldSim code read log(I) for 50%<RH, when they should read log(I) for RH<50%. Third, the I_drip_case3c look-up table, when compared with Table 6-15 in CRWMS M&O (2000c), replaces the 1-R^{es} values "<0.001" and "0.001" with "0.001199" and "0.0012," respectively (R^{es} is the ratio of the evaporation flow rate and the seepage flow rate).

While Ionic_Str_Invert is consistent with the description in the TSPA–SR model report, it is not clear if it is faithful to the model abstraction for invert ionic strength described CRWMS M&O, 2000k). This discrepancy is discussed in Subsection 3.4.2.3.2.

3.4.1.4.4 pH_Invert

The selector pH_Invert, which assigns the invert pH value based on relative humidity, is implemented consistently with CRWMS M&O (2000c). This selector is dependent on three others—pH_invert_bound, pH_drip_case2, and pH_drip_case3—that are also reviewed in this report (Table 3-4: Subsections 3.4.1.4.1, 3.4.1.4.2, and 3.4.1.4.5).

Although pH_Invert is consistent with the description in the TSPA–SR model report, it is not clear if it is faithful to the model abstraction for invert pH described in CRWMS M&O (2000k). This discrepancy is discussed in Subsection 3.4.2.3.2.

3.4.1.4.5 pH_drip_case3

This selector defines the in-drift pH for relative humidities above 85 percent. The three look-up tables to which it points—pH_drip_case3a, pH_drip_case3b, and pH_drip_case3c—were also checked. The TSPA–GoldSim code implementation is consistent with the model and data references (Table 3-4) with two differences (probably not relevant): the pH_drip_case3c look-up table, when compared with Table 6-15 in CRWMS M&O (2000c), replaces the 1-R^{es} values "<0.001" and "0.001" with "0.001199" and "0.0012," respectively.

3.4.1.4.6 One-Dimensional Tables

Two colloid-relevant one-dimensional table elements were checked during the review—KC_PU_GW_COLLOID and KC_AM_GW_COLLOID (Table 3-4). These are representations of the K_c parameter, which is used to model transport via reversible attachment to colloids, for plutonium and americium (CRWMS M&O, 2000c,n). Both elements are included in the TSPA–GoldSim code input file, however, only KC_AM_GW_COLLOID is used. The reason for using the sorption coefficient of americium, K_c, is that americium yields the highest sorption coefficients in colloid experiments (CRWMS M&O, 2000n). It is, therefore, conservative to use the americium value for other radioelements such as plutonium. In the TSPA–GoldSim code, the values listed in the KC_AM_GW_COLLOID table were found to be lognormally distributed with a geometric mean of 0.003 and standard deviation of 10.2. These

distribution parameters match the statistics for K_c reported in CRWMS M&O (2000n, p. 56). Therefore, KC_AM_GW_COLLOID was correctly implemented in the TSPA–GoldSim code.

3.4.2 Model Implementation

3.4.2.1 Scope of Review

This review included TSPA–GoldSim code implementation of colloid release modeling, including release and transport within the waste package and invert. The text reviewed was Subsection 6.3.4.6, Colloids, in CRWMS M&O (2000c). Therefore, the review emphasized the calculations of masses of colloids and colloid-associated radionuclides as functions of in-package and in-drift chemistry. The discussion of Results and Verification (CRWMS M&O, 2000c, pp. 331–333) was checked directly by comparing the resulting time-dependent concentrations of colloids and colloidal plutonium against those expected based on the plots, algorithms, and equations in the colloid release analyses and model reports (CRWMS M&O, 2000k,l). The review relied on other subsections of Section 6.3.4, and on portions of Section 6.3.2, Near-Field Environment of CRWMS M&O (2000c) for supplemental information on modeled in-package and in-drift pH and ionic strength. Section 6.3.5, Engineered Barrier Transport, of CRWMS M&O (2000c) contains some discussion of invert colloid transport modeling, however, this section was not reviewed because no model results were discussed in that section.

This review was intended to verify that the TSPA–GoldSim code correctly implements the model described in CRWMS M&O (2000b,c) and that the model correctly implements the process model abstractions developed in supporting analyses and model reports (CRWMS M&O, 2000k,l). This review did not address the validity of the technical bases for the models; that type of review has been documented in ongoing interactions with DOE (NRC, 2002b).[1,2,3] The earlier reviews identified several model development and implementation issues, such as the link between colloid concentration uncertainty and chemistry uncertainty, the selection of release and transport parameters, the hand-off of colloidal mass throughout the transport pathway, and the selection of radionuclides for colloid modeling. The exclusion of these issues from this report is not meant to imply those issues are resolved. The present review is narrowly focused on the implementation of the abstractions as developed and does not extend to colloid transport models below the drift.

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[1]Reamer, C.W. "U.S. Nuclear Regulatory Commission/U.S. Department of Energy Technical Exchange and Management Meeting on Evolution of the Near-Field Environment (January 9–12, 2001)." Letter (January 26) to S. Brocoum, DOE. Washington, DC: NRC. 2001a.

[2]Reamer, C.W. "U.S. Nuclear Regulatory Commission/U.S. Department of Energy Technical Exchange and Management Meeting on Radionuclide Transport (December 5.7,2000). Letter (December 12) to S. Brocoum, DOE. Washington, DC: NRC. 2000.

[3]Reamer, C.W. "U.S. Nuclear Regulatory Commission/U.S. Department of Energy Technical Exchange and Management Meeting on Total System Performance Assessment and Integration (August 6–10, 2001)." Letter (August 23) to S. Brocoum, DOE. Washington DC: NRC. 2001b.

3.4.2.2 Model Highlights

Colloid-associated radionuclide release is modeled as resulting from both reversible and irreversible attachment of radionuclides to colloids (CRWMS M&O, 2000b,c,k,l,) as functions of chemistry in the waste package. The total system performance assessment model calculates water concentrations of (i) radionuclides irreversibly attached to waste form colloids, (ii) waste form colloids, (iii) corrosion product iron oxyhydroxide (iron-oxide) colloids, (iv) groundwater colloids, and (v) radionuclides reversibly attached to waste form, iron-oxide, and groundwater colloids. The same calculations are repeated for the invert using modeled in-drift conditions. The underlying geochemical principles employed, supported by laboratory and field data, include the effects of solution pH and ionic strength on colloid stability and equilibrium sorption of dissolved radionuclides onto colloids.

3.4.2.3 Review Findings

In general, the TSPA–GoldSim code model implementation for colloid release and transport in the engineered barrier subsystem was consistent with the model abstraction analyses and model reports. Exceptions are discussed in the following subsections. Integration with the unsaturated and saturated zone colloid transport implementation was not reviewed, however, it is a continuing source of interest and discussion.[4]

3.4.2.3.1 Condition B

Condition B is a logic statement that is part of the calculation of iron-oxide colloid concentration in both the waste package and invert; the TSPA–GoldSim code expressions are condition_B_WP and condition_B_invert. These expressions directly affect whether the iron-oxide colloid concentration is set to a minimum value of 0.001 mg/l [8.3×10^{-9} lb/gal] or a maximum value of 1 mg/l [8.3×10^{-9} lb/gal] (CRWMS M&O, 2000l). The iron-oxide colloid concentration, in turn, directly affects the concentration of reversibly attached radionuclides; that is, selection of the maximum concentration results in a concentration of radionuclides reversibly attached to iron-oxide colloids that is 1,000 times higher than if the minimum value were selected. During the model input review, it was found that condition_B_WP and condition_B_invert faithfully reflect the intended abstractions (CRWMS M&O, 2000l, Figure 15e; 2000k, Figure 8), however, the condition was stated incorrectly in the abstractions.

For convenience, only those instances of Condition B in the CDSP_Packages\Infiltration_Bin_3\Intermittent_Drip portion of the TSPA–GoldSim code will be discussed, however, all instances of Condition B have the same error. The condition_B_WP and condition_B_invert expressions:

> if(Ionic_Str_CDSP>((-0.02*pH_CDSP)+0.17) **OR** Ionic_Str_CDSP >((0.02*pH_CDSP)-0.17),1,0)

and

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[4]Reamer, C.W. "U.S. Nuclear Regulatory Commission/U.S. Department of Energy Technical Exchange and Management Meeting on Total System Performance Assessment and Integration (August 6–10, 2001)." Letter (August 23) to S. Brocoum, DOE. Washington DC: NRC. 2001b.

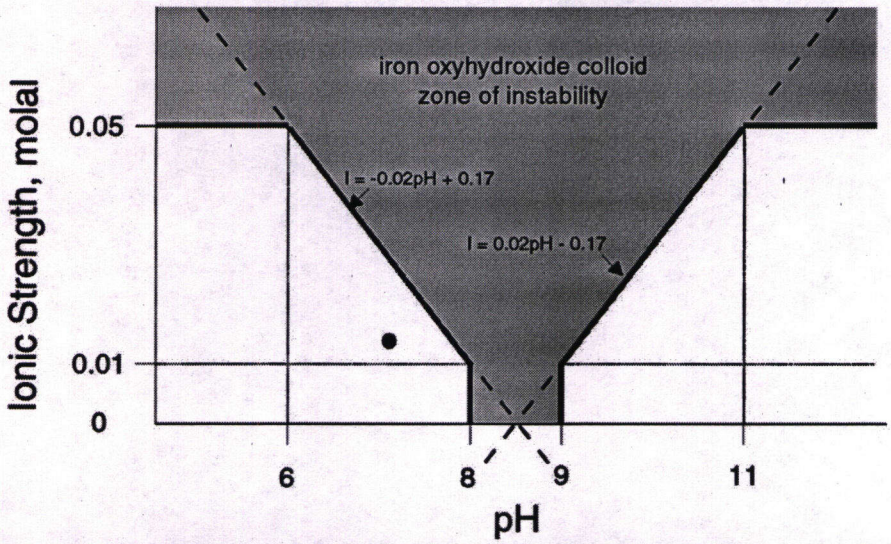

Figure 3-13. Iron_Oxide Colloid Stability Diagram, Showing the Two Lines (Dashed) Represented by Condition B. the Solid Dot Represents Conditions at 100,000 Years for the Median Value Case.

if(Ionic_Str_invert>((-0.02*pH_invert)+0.17) **OR** Ionic_Str_invert >((0.02*pH_invert)-0.17),1,0)

Condition B is represented graphically in Figure 3-13, which is modified from Figure 11 in CRWMS M&O (2000l) and is also reproduced as Figure 7 in the CRWMS M&O (2000k). In combination with Condition A, Condition B is intended to set the iron-oxide colloid mass to its minimum value if pH and ionic strength lie in the shaded zone of instability. The intended abstraction is that if ionic strength is between the upper and lower threshold values of 0.01 and 0.05 molal (Condition A) and above the two sloping lines between pH 6 and 8 and between pH 9 and 11, iron-oxide colloids are unstable, and the minimum concentration will be selected. The two sloping lines are represented by the equations $I = -0.02*pH + 0.17$ and $I = 0.02*pH - 0.17$. It can be seen in Figure 3-13 that the condition that ionic strength be above one line or the other applies to all positive values of ionic strength because the lines intersect on the zero axis. Therefore, Condition B will always be true (value of one in the TSPA–GoldSim code expressions), and the minimum iron-oxide colloid concentration will incorrectly be chosen for all conditions with ionic strength between 0.01 and 0.05 molal. The operator in Condition B should be AND. For example, a correct expression for condition_B_WP would be

if{Ionic_Str_CDSP>[(-0.02*pH_CDSP)+0.17] AND Ionic_Str_CDSP >[(0.02*pH_CDSP)-0.17],1,0}.

The effect of this error on calculated colloid concentration was illustrated in Results and Verification, Section 6.3.4.6, Colloids, of CRWMS M&O (2000c, p. 332), where it was concluded that invert iron-oxide colloid concentration after waste package failure will be at the minimum

value at later times because Condition B is true (CRWMS M&O, 2000c, Figure 6-144). In the median value case used for results and verification in CRWMS M&O (2000c), the modeled pH for 100,000 years is 7.07 (p. 192), and the ionic strength is 0.0145 molal (p. 191 and Figure 6-143). Figure 6-144 of CRWMS M&O (2000c) shows the iron-oxide colloid concentration at the minimum value at this time. This point is plotted in pH-ionic strength space on Figure 3-13, however, and is clearly in the zone of stability. The error in Condition B ensures iron-oxide colloid concentration in the waste package or the invert will always be at the minimum when ionic strength is between 0.01 and 0.05 molal and that, therefore, the mass of reversibly attached radionuclides in the waste package and invert will be underestimated for those conditions wherein they should be stable.

3.4.2.3.2 Invert Water Chemistry

In Sections 3.4.1.4.3 and 3.4.1.4.4, it was reported that the selectors Ionic_Str_Invert and pH_Invert were not consistent with the relevant abstraction analyses and model report (CRWMS M&O, 2000k). Figure 3 and Table 1 from this analyses and model report show that ionic strength and pH in the invert are intended to be calculated as a mixture between water coming from the waste package and ambient groundwater (CRWMS M&O, 2000k). The site recommendation model and the TSPA–GoldSim code implementation does not include this mixing process and, instead, hands off to the invert the chemistry calculated for the in-drift environment using the precipitates/salts approach (CRWMS M&O, 2000m,p). For colloid calculations, the performance assessment model approach may not be conservative because any addition of a groundwater component to in-drift water is likely to lower the ionic strength. Lower ionic strength tends to stabilize colloids. Also, in the performance assessment model, in-drift pH affects not only calculated invert colloidal concentrations, but is also a factor in solubility calculations for uranium, neptunium, and americium in the invert (CRWMS M&O, 2000c, pp. 310–312). A technical basis is lacking for the use in the invert of water chemistries calculated with the precipitates/salts models.

The present review does not address issues of the technical bases for the in-package and in-drift chemical models employed in the performance assessment model. Previous NRC reviews have been conducted, and outstanding issues remain (NRC, 2002b).

3.4.2.3.3 Tracking Colloid-Associated Radionuclide Mass

One aspect of colloid-associated transport within the engineered barrier subsystem that was not transparent during this review was the fate of a radionuclide mass as a result of changes in calculated mass between the waste package and invert. Because masses of colloids and colloidal radionuclides are recalculated for the modeled chemical conditions in the invert, significant amounts of radionuclides may be lost or gained in this transition. Furthermore, because of the extreme sensitivity of calculated masses to chemical conditions, these changes can be large. Whether or not these lost or gained masses are accounted for was not clear from this review of the TSPA–GoldSim code and is a continuing source of lack of transparency how the models function. This uncertainty also applies to the hand-off of colloidal radionuclides to the unsaturated zone, which was not reviewed.

3.4.3 Summary

Various errors and deficiencies were found among the 41 TSPA–GoldSim code model input elements reviewed.

- In expression Mass_Pu239_Irrev, the mass units apparently are inconsistent and would yield an incorrect result. This error may also affect analogous expressions for other radionuclides.

- Data element CPu_Col_Wf_Irrev_max, which is the maximum value for the concentration of irreversibly attached plutonium, is given a value {6×10^{-8} mol/l [2.3×10^{-7} mol/gal]} that is lower than that assigned in the supporting analyses and model report {8×10^{-8} mol/l [3×10^{-7} mol/gal]} on the basis of laboratory data.

- No technical basis has been provided for the values assigned to data elements M_Col_Feox_max and M_Col_Feox_min.

- The lognormal distributions for the three americium colloid sorption coefficients (Kd_wf_coll_Am, Kd_gw_coll_Am, and Kd_fe_coll_Am) were altered to truncated lognormal distributions in the TSPA–GoldSim code.

- The derivation of the six reviewed stochastic elements (Kd_wf_coll_Pu, Kd_gw_coll_Pu, Kd_fe_coll_Pu, Kd_wf_coll_Am, Kd_gw_coll_Am, and Kd_fe_coll_Am) was not transparent and easily traceable, and the use of this stochastic elements was not justified in light of evidence for kinetic effects on sorption to colloids.

- Selector pH_invert_bound assigns the wrong bounding pH values for times between 1,000 and 100,000 years.

- Time periods used in selector element pH_drip_case2 differ by 50 years from those in CRWMS M&O (2000TSPA Model) and elsewhere in the TSPA–GoldSim code.

- The I_drip_case3 and pH_drip_case3 look-up tables substitute the $1\text{-}R^{es}$ values "<0.001" and "0.001" with "0.001199" and "0.0012," respectively.

Although it is clear that some input deviations (e.g., the $1\text{-}R^{es}$ and CPu_Col_Wf_Irrev_max values) are not likely to introduce significant model errors, others (e.g., pH_invert_bound selector) may. In addition, because this review included only a small number of model elements, the identified errors point to the possibility of unidentified others that may be more significant.

Three model implementation issues were identified during this review.

- Expression condition_B_WP and analogous Condition B expressions in the TSPA–GoldSim code inherited an algorithm error from the model abstraction analyses and model report. This error causes the minimum iron-oxide colloid concentration to be erroneously selected for all conditions under which the ionic strength is between 0.01 and 0.05 molal. The effect of this error is pronounced because the maximum and

minimum concentrations, one of which is selected with no intermediate value, differ by a factor of 1,000. (This large sensitivity of colloid concentrations to modeled chemical conditions is the subject of a DOE and NRC agreement).[5]

- The TSPA–GoldSim code in-drift chemical model implemented by selectors Ionic_Str_Invert and pH_Invert neglects the mixture of ambient groundwater proposed in the model abstraction analyses and model report. Rather, the TSPA–GoldSim code for the invert applies pH and ionic strength calculated with the precipitates/salts approach, with no potential for dilution by groundwater. This may result in underestimation of colloid concentrations (and, perhaps, radionuclide solubilities) in the invert relative to the original abstraction.

- Tracking of colloid and colloidal radionuclide mass between the waste package and invert is not transparent.

3.5 Biosphere

The biosphere modeling in the DOE TSPA–GoldSim code model represents human exposure pathways and exposure scenarios in the accessible environment that convert estimated concentrations of radionuclides in groundwater to human doses. The biosphere modeling also sums groundwater concentrations to produce results consistent with groundwater protection limits in 10 CFR Part 63 (NRC, 2001). Review of the DOE biosphere modeling in the TSPA–GoldSim code included an input data review for traceability and a verification review to check model implementation.

3.5.1 Model Input

The input data review was conducted to check the data in the SR00_037ne6.gsm file of the TSPA–GoldSim code biosphere model can be traced to and verified against applicable documentation. The expressions, data, and stochastic inputs checked during the input review are listed in Table 3-5.

The expressions Annual_Water_Usage, A, and the stochastic data for R1 and R2 are used in the groundwater concentration calculations. A is an expression that computes an annual usage rate per farm. Annual_Water_Usage is calculated from the product of A and R2, which is a stochastic variable representing the number of farms. The definition for A in the TSPA-GoldSim code median case file (SR00_037ne6.gsm) is

$$A = 96.92\,\text{acre ft / yr} + R1 \times 37.77\,\text{acre ft / yr} \qquad (3\text{-}16)$$

The value 96.92 acre-ft/yr was traced to the DOE documentation for the Site Recommendation (CRWMS M&O, 2000b) and a supporting analysis and model report on water usage (CRWMS M&O, 2000q) as the mean annual water usage per farm based on active water permits in 1997. The value of 37.77 acre-ft/yr in Eq. (3-16) was found in the same sources (CRWMS M&O, 2000b,q) as the uncertainty in mean water usage (when added and subtracted

[5]Reamer, C.W. "U.S. Nuclear Regulatory Commission/U.S. Department of Energy Technical Exchange and Management Meeting on Total System Performance Assessment and Integration (August 6–10, 2001)." Letter (August 23) to S. Brocoum, DOE. Washington DC: NRC. 2001b.

Table 3-5. Reviewed TSPA–GoldSim Code Expressions and Stochastic Elements Related to Biosphere	
Expression	**References**
Annual_Water_Usage	CRWMS M&O, 2000b,c,q,r
A	CRWMS M&O, 2000b,c,q,r
Stochastic	**References**
BDCF_Tc99	CRWMS M&O, 2000b,r,s,t
BDCF_I129	CRWMS M&O, 2000b,r,s,t
BDCF_Am241	CRWMS M&O, 2000b,r,s,t
BDCF_Np237	CRWMS M&O, 2000b,r,s,t
BDCF_Pu239	CRWMS M&O, 2000b,r,s,t
R1	CRWMS M&O, 2000b,c,q,r
R2	CRWMS M&O, 2000b,c,q,r; NRC, 1999

from the mean value, this number represents the ends of the 95-percent confidence interval for the water usage data). In the SR00_037ne6.gsm file, the value of stochastic variable R1 is sampled from uniform distribution ranging from -1 to 1. Finally, R2, the number of farms, is also uniformly distributed in the range 15 to 25 in the SR00_037ne6.gsm file. This range and distribution for the number of farms were traced to the DOE documentation (referencing supplementary information in the proposed rule for 10 CFR Part 63 (NRC, 1999) that states 15 to 25 farms is representative of current conditions of the region. The number of farms was confirmed also to be consistent with the final rule for 10 CFR Part 63 (NRC, 2001). Considered together, the annual water usage was confirmed to be calculated in the TSPA–GoldSim code as a stochastic parameter that varies about the mean annual farm usage estimate by a variable number of farms and the 95-percent confidence interval about the mean estimated annual water use. The review of the Annual_Water_Use expression and its associated expressions and input data confirmed correct implementation and consistency with the supporting DOE documentation.

The biosphere dose calculation model is an abstraction of pathway modeling conducted outside the TSPA–GoldSim code model. Primary inputs to the TSPA–GoldSim code model are the stochastic Biosphere Dose Conversion Factors (e.g., BDCF_Am241) that convert concentrations in soil and groundwater to dose. Table 3-6 shows a comparison of biosphere dose conversion factor inputs in the TSPA–GoldSim code. Here, the parameters needed to define the parameter distribution, the geometric mean and geometric standard deviation, were compared for selected radionuclides with the values reported in CRWMS M&O (2000b) and traced from there to the supporting DOE documentation (CRWMS M&O, 2000r; CRWMS M&O, 2000s; CRWMS M&O, 2000t). Values in the SR00_037ne6.gsm file and the supporting documentation were found to be consistent with one exception. The biosphere dose conversion factor for I-129 in a supporting analysis and model report (CRWMS M&O, 2000t, Table 9) was a

factor of 10 higher than the value reported in prior (CRWMS M&O 2000s) and subsequent (CRWMS M&O, 2000r) DOE documentation for the result. This was, therefore, presumed to be a typographical error of no significance to the TSPA–GoldSim code model. Additional checking of the TSPA–GoldSim code median case BDCF value (SR00_037ne6.gsm file) was accomplished and results are provided in Table 3-7. Table 3-7 shows biosphere dose conversion factors in the TSPA–GoldSim code match values found in CRWMS M&O (2000b).

The GENII-S (Leigh, et al., 1993) modeling that generated the biosphere dose conversion factors relies on substantial input data. These data were not included in this review because they were previously reviewed to support a 2001 total system performance assessment technical exchange that resulted in comments to DOE and related agreements.[6] In addition, an external input review was not conducted because no dynamic linked libraries were used in the DOE biosphere model.

3.5.2 Model Implementation

Implementation of the biosphere calculations was also reviewed. Because the biosphere calculations are abstractions of modeling conducted outside the TSPA–GoldSim code, the calculations in the TSPA–GoldSim code are simple operations that were checked by hand calculations.

3.5.2.1 Scope of Review

All elements in the biosphere container were initially reviewed to develop an understanding of the nature and scope of the calculations. Primary emphasis was placed on the total dose function (Total_Dose) and the groundwater protection calculations in the container labeled GWPC_Results. These calculations were traced back through related calculations to the point where groundwater concentrations are passed to the biosphere model from the saturated zone model. Calculations were verified by hand calculations for a sample of radionuclides. Specific calculations checked include the average individual dose function (Avg_Ind_Dose), the average individual dose for groundwater protection function (Avg_Individual_Dose_GWPC), the gross alpha activity function (Gross_Alpha_Activity), and the combined radium concentration function (Concentration_Ra226_Ra228).

3.5.2.2 Model Highlights

The DOE biosphere process model converts estimated concentrations of radionuclides in groundwater (Conc_Curies_20km) to radiation doses (Avg_Ind_Dose and Total_Dose) necessary for demonstrating compliance with the individual dose limit in 10 CFR Part 63 (NRC, 2001). The model also produces groundwater concentrations (Conc_Curies_20km_GWPC, Concentration_Ra226_Ra228, and Gross_Alpha_Activity) in a form necessary for demonstrating compliance with groundwater protection requirements in 10 CFR Part 63 (NRC, 2001).

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[6]Reamer, C.W. "U.S. Nuclear Regulatory Commission/U.S. Department of Energy Technical Exchange and Management Meeting on Total System Performance Assessment and Integration (August 6–10, 2001)." Letter (August 23) to S. Brocoum, DOE. Washington DC: NRC. 2001b.

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Table 3-6. Comparison of Groundwater Biosphere Dose Conversion Factor Lognormal Parameter Distribution Data in the TSPA–GoldSim Code with the DOE Documentation

Radionuclide	Biosphere Dose Conversion Factor Data from the SR00_037ne6.gsm File (mrem/yr per pCi/L)†		Biosphere Dose Conversion Factor Data from the DOE Documentation* (mrem/yr per pCi/L)†	
	Geometric Mean	Geometric Standard Deviation	Geometric Mean	Geometric Standard Deviation
Tc-99	1.49E-03	1.84	1.49E-03	1.84
I-129	3.56E-01	1.19	3.56E-01	1.19
Np-237	6.74E+00	1.16	6.74E+00	1.16
Pu-239	4.98E+00	1.15	4.98E+00	1.15
Am-241	5.01E+00	1.16	5.01E+00	1.16

*CRWMS M&O, 2000b
†English units are not provided to keep consistency with source documents.

Table 3-7. Comparison of Groundwater Biosphere Dose Conversion Factors in the SR00_037ne6.gsm File with the DOE Documentation

Radionuclide	Biosphere Dose Conversion Factors (mrem/yr per pCi/L)‡		
	DOE Documentation* (geometric mean)	File SR00_037ne6.gsm	Ratio
C-14	4.02E-03†	4.02E-03	1.00
Tc-99	3.66E-03†	3.66E-03	1.00
I-129	3.56E-01	3.56E-01	1.00
Ac-227	1.80E+01	1.80E+01	1.00
Th-229	5.39E+00	5.39E+00	1.00
U-232	2.06E+00	2.06E+00	1.00
U-233	3.85E-01	3.85E-01	1.00
U-234	3.77E-01	3.77E-01	1.00
U-236	3.56E-01	3.56E-01	1.00
U-238	3.51E-01	3.51E-01	1.00
Np-237	6.74E+00	6.74E+00	1.00
Pu-238	4.11E+00	4.11E+00	1.00
Pu-239	4.98E+00	4.98E+00	1.00
Pu-240	4.95E+00	4.95E+00	1.00
Am-241	5.01E+00	5.02E+00	1.00
Am-243	5.03E+00	5.03E+00	1.00

*CRWMS M&O, 2000b
†Values for Tc-99 and C-14 reported in table have been adjusted for a shifted distribution as described in the DOE documentation.
‡English units are not provided to keep consistency with source documents.

Groundwater concentrations are calculated by first obtaining the product of mass radionuclide species flux from the saturated zone (SZOUT.Water_to_Sink) and the specific activity of each radionuclide (Specific_Activity vector). The result is then divided by the amount of water use (Annual_Water_Usage for individual protection or GWPC_Fixed_Water_Volume for groundwater protection) to produce groundwater concentrations for each radionuclide (Conc_Curies_20km and Conc_Curies_20km_GWPC). For comparison with groundwater protection limits, subgroups of radionuclide concentrations are summed to produce gross alpha activity (Gross_Alpha_Activity) and combined radium activity (Concentration_Ra226_Ra228).

Dose calculations are executed first for individual radionuclide species (Avg_Ind_Dose and Avg_Individual_Dose_GWPC), and resulting doses are summed to produce a total dose from all radionuclides (Total_Dose and Total_Dose_GWPC). Doses are calculated by obtaining the product of radionuclide concentrations in groundwater (Conc_Curies_20km and Conc_Curies_20km_GWPC) and applicable biosphere dose conversion factors (BDCF for individual protection limit and BDCF_Nominal_GWPC for groundwater protection dose limit).

The use of biosphere dose conversion factors (BDCF and BDCF_Nominal_GWPC) is an abstraction of modeling that accounts for a variety of transport and exposure pathways in the biosphere of the Yucca Mountain region. The pathway dose modeling is accomplished by executing the GENII-S code (Leigh, et al., 1993) outside the TSPA–GoldSim code model for unit concentrations of radionuclides in the groundwater. The resulting biosphere dose conversion factors (BDCF, BDCF_Nominal_GWPC) are used as stochastic inputs to the TSPA–GoldSim code that are sampled each realization for use in the aforementioned dose calculations. NRC previously reviewed the DOE implementation of the biosphere dose conversion factor sampling approach and has discussed concerns with DOE at a technical exchange that generated an issue resolution agreement (TSPAI.3.37).[7] DOE has recently provided a response.[8] to the concerns raised in the agreement, and staff are currently reviewing this DOE response and plan to submit a response letter. To avoid unnecessary duplication, the issues related to this agreement are not discussed further in this report.

3.5.2.3 Review Findings

Results and data used for verification of selected calculations are provided in Tables 3-8 through 3-11. Table 3-8 presents data extracted from the TSPA–GoldSim code median case (file SR00_037ne6.gsm) used to calculate the groundwater concentrations for the individual dose calculations. When the flux from the saturated zone (SZOUT.Water_To_Sink) is multiplied by the specific activity and divided by the annual water use, the result is the groundwater concentration at 20 km [12.4 mi] (Conc_Curies_20km). This check provides confidence that the TSPA–GoldSim code is correctly passing the information from the saturated zone model to the biosphere and that the concentration calculation is being implemented as expected.

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[7]Reamer, C.W. "U.S. Nuclear Regulatory Commission/U.S. Department of Energy Technical Exchange and Management Meeting on Total System Performance Assessment and Integration (August 6–10, 2001)." Letter (August 23) to S. Brocoum, DOE. Washington DC: NRC. 2001b.

[8]Ziegler, J.D. "Transmittal of Report Addressing Key Technical Issue (KTI) Agreement Item Total System Performance Assessment and Integration (TSPAI) 3.37," Letter (August 29, 2002) to J.R. Schlueter, Division of Waste Management, Office of Nuclear Materials Safety and Safeguards, NRC. Washington DC: DOE. 2002.

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Table 3-8. Data for Verification of Groundwater Well Concentration Calculation for Individual Protection Limit				
Radionuclide	SZOUT.Water_To_Sink (g/yr)*	Specific_Activity (Ci/g)*	Annual_Water_Usage (L/yr)*	Conc_Curies_20km (pCi/L)*
Tc-99	1.35E-02	1.69E-02	2.39E+09	9.58E-02
I-129	1.91E-02	1.63E-04	2.39E+09	1.30E-03
Np-237	1.53E+00	7.05E-04	2.39E+09	4.52E-01

*English units are not provided to keep consistency with source documents.
Note: Data have been rounded to three significant digits for presentation, however, verification calculations included all digits from the TSPA–GoldSim code input data.

Table 3-9 provides information necessary to verify the calculation of dose for comparison with the individual protection limits in 10 CFR Part 63 (NRC, 2001). This calculation uses the groundwater concentration (Conc_Curies_20km) verified in Table 3-8 and multiplies by the applicable biosphere dose conversion factor (BDCF) to obtain the average individual dose for each radionuclide (Avg_Ind_Dose). The results of the hand calculation agree with the dose values found in the TSPA–GoldSim code median case (file SR00_037ne6.gsm). This result provides confidence the average individual dose calculation in the TSPA–GoldSim code is being implemented as expected.

Table 3-10 presents data extracted from the TSPA–GoldSim code median case (file SR00_037ne6.gsm) used to calculate the groundwater concentrations for the groundwater protection calculations. When the flux from the saturated zone (SZOUT.Water_To_Sink) is multiplied by the specific activity and divided by the fixed water volume from proposed regulations in 10 CFR Part 63 (NRC, 1999)(GWPC_Fixed_Water_Volume), the result is the groundwater concentration at 20 km [12.4 mi] (Conc_Curies_20km_GWPC). This check provides confidence that the TSPA–GoldSim code is correctly passing the information from the saturated zone model to the biosphere and that the concentration calculation is being implemented as expected. Note the value for the fixed water volume is based on proposed regulations that have been superseded by recently promulgated final regulations in 10 CFR Part 63 (NRC, 2001) that have a new value for this parameter. Staff will monitor future iterations of the DOE TSPA–GoldSim code implementation to ensure the data have been changed to be consistent with the final regulations in 10 CFR Part 63 (NRC, 2001).

Table 3-11 provides information necessary to verify the calculation of dose for comparison with the groundwater protection limits in 10 CFR Part 63 (NRC, 2001). This calculation uses the groundwater concentration (Conc_Curies_20km_GWPC) that was verified in Table 3-10 and multiplies it by the applicable biosphere dose conversion factor (BDCF_Nominal_GWPC) to obtain the average individual dose for each radionuclide (Avg_Individual_Dose_GWPC). The results of the hand calculation agree with the dose values found in the TSPA–GoldSim code median case (file SR00_037ne6.gsm). This result provides confidence that the average individual dose calculation in the TSPA–GoldSim code is being implemented as planned. The approach implemented in the version of the model reviewed, however, needs to be updated to reflect changes in the final regulations in 10 CFR Part 63 (NRC, 2001). For example, future

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Table 3-9. Verification of Individual Protection Dose Calculations the in TSPA–GoldSim Code

Radionuclide	Conc_Curies_20km (pCi/L)*	BDCF (mrem/yr per pCi/L)*	Avg_Ind_Dose (mrem/yr)*	Hand Calculated Individual Dose (mrem/yr)*
Tc-99	9.58E-02	3.66E-03	3.50E-04	3.50E-04
I-129	1.30E-03	3.56E-01	4.64E-04	4.64E-04
Np-237	4.52E-01	6.74E+00	3.05E+00	3.05E+00

*English units are not provided to keep consistency with source documents.
Note: Data have been rounded to three significant digits for presentation, however, calculations included all digits from the TSPA–GoldSim Code input data.

Table 3-10. Data for Verification of Groundwater Well Concentration Calculation for Groundwater Protection Limit

Radionuclide	SZOUT.Water_To_Sink (g/yr)*	Specific_Activity (Ci/g)*	GWPC_Fixed_Water_Volume (L/yr)*	Conc_Curies_20km_GWPC (pCi/L)*
Tc-99	1.35E-02	1.69E-02	1.59E+09	1.44E-01
I-129	1.91E-02	1.63E-04	1.59E+09	1.96E-03
Np-237	1.53E+00	7.05E-04	1.59E+09	6.80E-01

*English units are not provided to keep consistency with source documents.
Note: Data have been rounded to three significant digits for presentation, however, calculations included all digits from the TSPA–GoldSim code input data.

Table 3-11. Verification of Groundwater Protection Dose Calculations in the TSPA–GoldSim Code Median Case (SR00_037ne6.gsm File)

Radionuclide	Conc_Curies_20k_GWPC (pCi/L)*	BDCF_Nominal_GWPC (mrem/yr per pCi/L)*	Avg_Individual_Dose_GWPC (mrem/yr)*	Hand Calculated Individual Dose (mrem/yr)*
Tc-99	1.44E-01	3.66E-03	5.26E-04	5.26E-04
I-129	1.96E-03	3.56E-01	6.98E-04	6.98E-04
Np-237	6.80E-01	6.74E+00	4.58E+00	4.58E+00

*English units are not provided to keep consistency with source documents.
Note: Data have been rounded to 3 significant digits for presentation but calculations included all digits from TSPA–GoldSim input data.

revisions should reflect an 18-km [11.2-mi] compliance location rather than the currently used 20-km [12.4-mi] location. The dose calculation for comparison with the groundwater protectio n standard in the final rulemaking for 10 CFR Part 63 (NRC, 2001) should be based on the drinking water pathway. Using the all pathway biosphere dose conversion factors for this calculation as appears in the reviewed model will overestimate the groundwater protection dose. Finally, there is no organ dose calculation for groundwater protection in the reviewed model. The final groundwater protection dose limit in 10 CFR Part 63 (NRC, 2001) applies to the whole body or any organ, therefore, both a whole body and organ doses should be calculated to demonstrate compliance.

Additional verifications involved the calculation of gross alpha activity and combined radium concentration for comparison with groundwater protection standards. The combined radium concentration calculation and the gross alpha activity calculation were straightforward, and no problems were identified. Hand calculations verified the summation of the radionuclide specific concentrations for the species included in the two groups (combined radon and gross alpha) is being implemented correctly.

3.5.3 Summary

The DOE biosphere model in the TSPA–GoldSim code was reviewed to verify selected input data matched supporting documentation. This review included input data related to the calculation of annual water usage and the biosphere dose conversion factor stochastic inputs. No discrepancies were identified between the input data in the TSPA–GoldSim code model and the supporting DOE documentation. An additional verification review checked the implementation of the biosphere calculations in the TSPA–GoldSim code model. This review included hand calculations of groundwater concentrations used for dose calculations relevant to individual protection and groundwater protection limits in 10 CFR Part 63 (NRC, 2001). Additional verification checks were accomplished on concentration calculations related to groundwater protection limits in 10 CFR Part 63 (NRC, 2001). No major problems were identified in the verification reviews, however, some aspects of the groundwater protection calculations need to be updated for consistency with recently promulgated final regulations in 10 CFR Part 63 (NRC, 2001). Some inconsistencies with the final standards include, use of a 20-km [12.4 mi] compliance boundary, use of the dilution volume from the proposed standards, use of the all pathway biosphere dose conversion factors for the groundwater protection dose calculation, and lack of an organ dose calculation to demonstrate compliance with the groundwater protection dose limit. DOE is planning to incorporate the final regulations into the TSPA–GoldSim code model and supporting DOE documentation in the future. Staff will continue to monitor the DOE progress in this area and review revised products when they are made available.

4 SUMMARY

This report documents review of specific submodels of the U.S. Department of Energy (DOE) total system performance assessment code implemented in the GoldSim code platform by inspecting the median-case run file named SR00_037ne6.gsm and supporting documentation. These review activities are consistent with review methods in NRC (2002) concerning the demonstration of compliance with the postclosure individual protection standard. The review focused on verifying the consistency between data, definitions, and algorithms in the SR00_037ne6.gsm file and the supporting DOE documentation. The review was split into two areas, model input and model implementation, consistent with a review outline developed by the NRC staff. For model input verification, a selected sample of data and expressions of the DOE TSPA–GoldSim code was traced to the source documents. Similarly, the model implementation review activity checked the appropriate function and representation of submodels in the TSPA–GoldSim code with respect to the DOE documentation.

The DOE total system performance assessment submodels reviewed included (i) the radionuclide inventory abstraction, (ii) igneous activity, (iii) waste package and drip shield degradations, (iv) colloid release and transport in the engineered barrier subsystem, and (v) the biosphere model. Submodels (i) and (ii) were reviewed for model input only. Model implementation review activities for submodels (iii), (iv), and (v) included constructing a simplified model to emulate the implementation of the general corrosion model; comparing colloid model verification results in the site recommendation document to outcomes predicted by process model abstraction reports; tracing information flow from the saturated zone model to the biosphere model; and verifying with hand calculations groundwater concentration, water usage, and dose estimates in the biosphere model. No inconsistencies were found in (ii). Inconsistencies between the DOE documentation and the TSPA–GoldSim implementation found in submodels (i), (iii), and (iv) related to lack of documentation or disagreement of parameter values and distributions and lack of correspondence in the model description. In (v), disagreement with the final release of 10 CFR Part 63 was noted; however, DOE is planning to incorporate final regulations into the TSPA–GoldSim code.

In the inventory abstraction, most radionuclide decay rate values in the SR00_037ne6.gsm file are lower than rates referenced CRWMS M&O (2000b). In general, inventory data for DOE-owned spent nuclear fuel and high-level waste in glass form in the inventory vectors of the SR00_037ne6.gsm file deviate significantly from the values in the supporting documentation. The latest revision of the inventory abstraction document (Bechtel SAIC Company, 2001) references source data only by title without any data identifier, making it difficult to identify the exact data used in the computations. Complete agreement was found in the igneous activity model between a selected set of data in the SR00_037ne6.gsm file and the DOE documentation.

For waste package and drip shield degradation models, no documentation was found for the definition of the parameter defining the number of cracks per patch, Cracks_per_Patch_Factor. Also, there is not enough documentation on the input vector, WAPDEG_inputs, to the general corrosion module. The vector, WAPDEG_inputs, contains more than 1,000 entries, without units or comments, making it difficult to trace any of its values to the DOE documentation. In the model implementation review activity, a simplified model to emulate the action of the method used by DOE to split distributions of corrosion rates into uncertainty and variability

contributions (referred to as the Gauss-Variance Partitioning method) was implemented, and adequate agreement with the DOE results was obtained. A simplified approach to emulate the general corrosion abstraction of the DOE total system performance assessment code was implemented. The waste package and drip shield degradation computations of the DOE performance assessment code are implemented in the form of an independent dynamic link library (known as the WAPDEG module, originally programmed in Fortran) that communicates with the TSPA–GoldSim code via input and output files. It was not possible to verify that the DOE general corrosion computations of the WAPDEG module were consistent with the DOE documentation, given the significant disagreement between simplified computations and results in the SR00_037ne6.gsm file.

In WAPDEG, the waste package and drip shield surfaces are discretized into patches, 1,000 and 500, respectively. The fraction of waste packages with at least one patch penetrated by general corrosion as a function of time seems dependent on the number of patches. There is disagreement between model definitions in the DOE documentation and the actual implementation in the TSPA–GoldSim code. One disagreement pertains to the definition for the fraction of degraded axial length for the waste package. This quantity is used as a factor to to estimate the amount of water available for radionuclide release. The definition implemented in TSPA–GoldSim code lacks physical meaning and is not consistent with the documentation (e.g., CRWMS M&O, 2000h). In a second disagreement, CRWMS M&O (2000b) states the fraction of degraded axial length for the drip shield is used as a factor to modify the seepage rate at the drift; however, the factor used in the TSPA–GoldSim code is the fraction of the surface corroded by general corrosion as a function of time. Figure 3-12 was created to visualize the effect of the noted inconsistencies. The approach described in CRWMS M&O (2000b,h) appears conservative with respect to the approach implemented in the TSPA–GoldSim code.

There is no clear description in the documentation on the relationship between the number of defects from the manufacturing defect abstraction model and the number of cracks from the slip-dissolution model. Also, there is no documentation on the effect of the number of patches on the waste package surface on the size of the area affected by stress corrosion cracking.

With respect to the colloid release and transport in the engineered barrier subsystem model, various errors and deficiencies were found among the 41 TSPA-GoldSim code model input elements reviewed. For example, in the expression, Mass_Pu239_Irrev, the mass units are apparently inconsistent and would yield an incorrect result. This error may also affect analogous expressions for other radionuclides. The data element, Cpu_Col_Wf_Irrev_max, which is the maximum value for the concentration of irreversibly attached plutonium, is given a value {6×10^{-8} mol/l [2.3×10^{-8} mol/gal]} lower than the value assigned {8×10^{-8} mol/l [3×10^{-7} mol/gal]} in the supporting analysis and model report (CRWMS M&O, 2000l) on the basis of laboratory data. No technical basis has been provided for the values of the data elements M_Col_Feox_max and M_Col_Feox_min. The lognormal distributions for the three americium colloid sorption coefficients (Kd_wf_coll_Am, Kd_gw_coll_Am, and Kd_fe_coll_Am) were altered to truncated lognormal distributions in the TSPA-GoldSim SR00_037ne6.gsm file. The derivation of the six reviewed stochastic elements (Kd_wf_coll_Pu, Kd_gw_coll_Pu, Kd_fe_coll_Pu, Kd_wf_coll_Am, Kd_gw_coll_Am, and Kd_fe_coll_Am) was not transparent and traceable, and their use was not justified in light of evidence for kinetic effects on sorption to colloids. The selector, pH_invert_bound, assigns the wrong bounding pH values for times between 1,000 and 100,000 years. The time periods used in selector element pH_drip_case2

differ by 50 years from those in the site recommendation model report (CRWMS M&O, 2000c) and also elsewhere in the SR00_037ne6.gsm file. The I_drip_case3 and pH_drip_case3 look-up tables contain values that slightly differ from source documents. Although it is clear that some input deviations are not likely to introduce significant model errors, others (e.g., the pH_invert_bound selector) may do so. In addition, because this review included only a small sample of model elements, the identified errors point to the possibility of undetected errors that may be more significant.

Three model implementation issues were identified during review of the submodel Colloid Release and Transport in the Engineered Barrier Subsystem. The expression, condition_B_WP, and analogous Condition B expressions in the SR00_037ne6.gsm file inherited an algorithm error from the model abstraction reports (CRWMS M&O, 2000k,l). This error causes the minimum iron-oxide colloid concentration to be erroneously selected for all conditions where the ionic strength is between 0.01 and 0.05 molal. The effect of this error is pronounced because maximum and minimum concentrations differ by a factor of 1,000. The TSPA-GoldSim code in-drift chemical model implemented by selectors Ionic_Str_Invert and pH_Invert neglects the mixture of ambient groundwater proposed in the model abstraction report (CRWMS M&O, 2000k). Rather, the TSPA–GoldSim code model for the invert applies pH and ionic strengths calculated with the precipitates/salts approach, with no potential for dilution by groundwater. This approach may result in underestimation of colloid concentrations (and, perhaps, radionuclide solubilities) in the invert relative to the original abstraction. Finally, tracking of colloid and colloidal radionuclide mass between the waste package and invert is not transparent in the TSPA–GoldSim code implementation.

In the DOE biosphere model, no discrepancies were identified between the input data in the TSPA–GoldSim code model and supporting documentation. Model implementation review activities included hand calculations of groundwater concentrations used for dose calculations relevant to individual protection and groundwater protection limits in 10 CFR Part 63 (NRC, 2001). Additional verification checks were performed on concentration calculations related to groundwater protection limits in 10 CFR Part 63 (NRC, 2001). No major problems were identified; however, some aspects of the groundwater protection calculations should be updated for consistency with recently promulgated final regulations in 10 CFR Part 63 (NRC, 2001). Inconsistencies with the final standards include use of a 20 km [12.4 mi] compliance boundary, use of the dilution volume from the proposed standards, use of the all pathway biosphere dose conversion factors for the groundwater protection dose calculation, and lack of an organ dose calculation to demonstrate compliance with the groundwater protection dose limit. DOE is planning to incorporate the final regulations into the TSPA–GoldSim code model and supporting documentation in the future.

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