OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
SPECIAL INSTRUCTION SHEET

Complete Only Applicable Items

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Page: 1 of: 1

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OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
CALCULATION COVER SHEET

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2. Calculation Title
Calculation of Probability and Size of Defect Flaws in Waste Package Closure Welds to Support WAPDEG Analysis

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DTN: MO9910SPAFWPWF.001 tracks source data.

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For TSPA-SR.

Revision History

10. Revision No.	11. Description of Revision
00	Initial issue.

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FIGURES

Page

1. PURPOSE

The purpose of this calculation is to document the abstraction process used to develop distributions representing the frequency of occurrence and size of flaws potentially found in waste package closure welds. This calculation supports Performance Assessment and was prepared under Technical Product Development Plan TDP-EBS-PA-000001 (Attachment I, DIRS 2). This calculation was developed in accordance with the AP-3.12Q *Calculations* procedure (AP-3.12Q, Rev. 0, ICN 0. *Calculations.* Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste management. ACC: MOL.19990702.0312).

2. METHOD

Flaw density and flaw size distributions are obtained from Analyses and Model Report (AMR) titled Analysis of Mechanisms for Early Waste Package Failure (Attachment I, DIRS 1). The flaw density is used as the parameter for a Poisson distribution used to represent the frequency of occurrence of flaws in a given length of closure weld. The flaw sizes are given as a probability density function on each closure weld.

3. ASSUMPTIONS

The following assumptions are made:

3.1 Only surface breaking flaws are considered, since these are the types of flaws that may potentially lead to stress corrosion cracking (SCC). The basis for this assumption is information from the Stress Corrosion Cracking model (Attachment I, DIRS 3). This assumption is used throughout the calculation.

3.2 Only the circumferential closure weld of the waste package develops residual stresses high enough to cause stress corrosion cracking (if a surface breaking flaw and aggressive environment are also present). Other welds used in waste package fabrication are annealed prior to waste emplacement, and thus do not develop residual stress magnitudes high enough to allow stress corrosion cracking to occur. The results of an improper annealing treatment are addressed elsewhere (Attachment I, DIRS 1, Sec. 6.2.3), and will not be considered in this calculation. This assumption is used throughout the calculation as in that only results for the closure weld are calculated.

3.3 Flaws are assumed to occur randomly as represented by a Poisson process. The Poisson process assumptions are listed in Section 5. These assumptions are reasonable for the manufacturing process being considered (Attachment I, DIRS 5). This assumption is used throughout this calculation.

3.4 The mean flaw density of 0.6839 flaws/meter (Poisson distribution parameter) of the closure weld is assumed to be as discussed in the Analysis of Mechanisms for Early Waste Package Failure (Attachment I, DIRS 1) and tracked by DTN: MO9910SPAFWPWF.001

(Attachment I, DIRS 6). This is a reasonable value based on the literature reviewed for the AMR. This assumption is used throughout this calculation.

3.5 The fraction of surface breaking flaws is assumed to be uniformly distributed between the minimum and maximum fractions (0.13% and 0.49% respectively) used to determine the average fraction quoted in Analysis of Mechanisms for Early Waste Package Failure (Attachment I, DIRS 1) and tracked by DTN: MO9910SPAFWPWF.001 (Attachment I, DIRS 6). The basis of this assumption is that the three values (0.13%, 0.40% and 0.49%) quoted in the AMR are not sufficient to determine a single representative average value. The use of the uniform distribution is a reasonable representation of the uncertainty in expressing this value. This assumption is used throughout this calculation.

3.6 Pre-inspection flaw sizes are assumed to be lognormally distributed, with distribution parameters (dependent on the weld thickness) as given in Analysis of Mechanisms for Early Waste Package Failure (Attachment I, DIRS 1) and tracked by DTN: MO9910SPAFWPWF.001 (Attachment I, DIRS 6). This assumption is used throughout the calculation.

3.7 The probability of non-detection (PND) is given as a function of flaw size in Analysis of Mechanisms for Early Waste Package Failure (Attachment I, DIRS 1, Sec. 6.2.1 and tracked by DTN: MO9910SPAFWPWF.001 (Attachment I, DIRS 6). The model is dependent on three parameters: the detection threshold (p), the location parameter (b), and a scale parameter (ν) (note that in the reference these parameters are γ, a^*, and ν respectively). The b and ν parameters are taken to be uncertain with a uniform distribution (1.6 to 5 mm and 1 to 3, respectively). The ranges for these distributions are determined from the values identified in the literature quoted in the Analysis of Mechanisms for Early Waste Package Failure (Attachment I, DIRS 1, Sec. 6.2.1) and tracked by DTN: MO9910SPAFWPWF.001 (Attachment I, DIRS 6). This is a reasonable assumption, as the manufacturing and detection processes for welds on the waste container are not specified to date. The best that may be modeled at this time are values based on similar industrial manufacturing practices as reviewed in Analysis of Mechanisms for Early Waste Package Failure (Attachment I, DIRS 1, Sec. 6.2.1) and tracked by DTN: MO9910SPAFWPWF.001 (Attachment I, DIRS 6). This assumption is used throughout the calculation.

3.8 It is assumed that all flaws detected are repaired to specified acceptance criteria or removed in such a manner that they are eliminated from consideration for further failure analysis. This assumption is used throughout the calculation.

4. USE OF COMPUTER SOFTWARE AND MODELS

The software used in this calculation include:

- Software Routine MFD, a Fortran subroutine to support the calculations presented in this document (see Attachment III, MFD Software Routine Report, for description and validation information). It is appropriate for the application and is used only within the range of validation.

- MathSoft Mathcad2000 Professional, commercially available software for technical calculations. This software is appropriate for this application as it offers the mathematical and graphical functionality necessary to perform and document the numerical manipulations used in this analysis. No applications or numerical manipulations of sufficient complexity to qualify as a software routine were implemented. Details of the Mathcad numerical manipulation performed in support of this document are discussed throughout this calculation.
- Microsoft Excel 97, commercially available spreadsheet software. This software was used as is, to graph results.

All software was executed on a DELL PowerEdge 2200 Workstation equipped with two Pentium II 266 MHz processors (CRWMS M&O tag 112517) in the Windows NT 4.0 operating system.

5. CALCULATION

Initial (pre-inspection) mean flaw densities and flaw sizes used in this calculation were supplied in by DTN: MO9910SPAFWPWF.001 (Attachment I, DIRS 6).

Calculation of the outer surface-breaking mean flaw density begins with the base mean flaw density of 0.6839 flaws/meter of weld for a one inch thick stainless steel Tungsten Inert Gas weld (this density was measured from an actual weld performed under shop conditions) subject to radiographic (RT) and dye-penetrant (PT) tests (Attachment I, DIRS 1, Sec. 6.2.1, and contained in DTN: MO9910SPAFWPWF.001 Attachment I, DIRS 6). To convert this value to a flaw density for an uninspected weld, the base flaw density is increased by the sum of the flaw reduction factors provided for the RT and PT tests. The adjustment for the RT exam increases the total flaw density by a factor of 12.8 while the PT exam, which detects only surface-breaking flaws, increases the density of only the surface-breaking flaws by a factor of 31.4 (Attachment I, DIRS 1, Sec. 6.2.1) (see DTN: MO9910SPAFWPWF.001 (Attachment I, DIRS 6)). Next the effect of weld thickness on flaw density is used to adjust for the actual weld thickness on the closure weld. For the 25-mm thick closure weld the flaw reduction factor (R) is 97.3% (865 divided by 889) (Attachment I, DIRS 1, Figure 6.2-1) (see DTN: MO9910SPAFWPWF.001 (Attachment I, DIRS 6)). Multiplying this result by this circumference of the closure weld results in the flaw density per closure weld (or per waste container). A final multiplication by the fraction of surface breaking flaws (Ψ) results in the final mean flaw density of surface breaking flaws per closure weld (λ). More generally,

$$\lambda = 0.6839 \cdot [12.8 + 31.4 \cdot \Psi] \cdot R(t) \cdot (2\pi r) \cdot \Psi$$

Where r is the radius of the closure lid (in meters), t is the weld thickness (in millimeters) and the flaw reduction factor $R(t)$ is given by,

$$R(t) = \begin{cases} \dfrac{-218 \cdot t + 5207}{2845}, & for \quad 6.35mm \le t \le 12.7mm \\ \dfrac{60 \cdot t - 635}{889}, & for \quad 19.05mm \le t \le 25.4mm \end{cases}.$$

For closure lid radius equal to 0.76 meters (DTN: MO9910SPAFWPWF.001),

$$\lambda(t,\Psi) = 3.2658 \cdot [12.8 + 31.4 \cdot \Psi] \cdot R(t) \cdot \Psi$$

the mean flaw density of surface breaking flaws per closure weld, λ, is a function of the lid thickness, t, and the fraction of surface breaking flaws, Ψ.

The initial (pre-inspection) flaw size distribution is assumed to be lognormal where the lognormal probability density function is given by

$$f(s) = \frac{1}{s\sigma\sqrt{2\pi}} exp\left[-\frac{1}{2\sigma^2}\left(ln\frac{s}{a_{50}}\right)^2\right] \qquad s > 0 .$$

Where s is the flaw size and the parameters, a_{50} and σ, are given as functions of weld thickness (t, in millimeters) as (Attachment I, DIRS 1, Sec. 6.2.1) (see DTN: MO9910SPAFWPWF.001 (Attachment I, DIRS 6)),

$$a_{50}(t) = 0.1159 \cdot 25.4 - 0.0445 \cdot t + \frac{0.00797}{25.4} \cdot t^2$$

$$\sigma(t) = 0.09733 + \frac{0.3425}{25.4} \cdot t - \frac{0.07288}{(25.4)^2} \cdot t^2 .$$

Here a_{50} is the median or geometric mean of the distribution and σ is the standard deviation of the natural log transformed flaw sizes (*ln(s)* values). For weld thickness equals to 25-mm the median value, a_{50} is equal to 2.027 and σ is equal to 0.364 (Attachment I, DIRS 1, Sec. 6.2.1) (see DTN: MO9910SPAFWPWF.001 (Attachment I, DIRS 6)). For weld thickness equals to 10-mm the median value, a_{50} is equal to 2.530 and σ is equal to 0.221.

Next the post-inspection mean flaw density and flaw size distribution must be calculated. The final closure weld is subject to an ultrasonic exam (UT) where the probability of non-detection (PND) is given as a function of flaw size. The PND function for this UT test is estimated to be (DTN: MO9910SPAFWPWF.001):

$$PND(s) = \left[\frac{p+1}{2} + \frac{p-1}{2} \cdot erf\left(v \cdot ln\left(\frac{s}{b}\right)\right)\right]^2$$

Where p is the lower limit of PND (0.005) (DTN: MO9910SPAFWPWF.001), *erf* is the error function, s is the flaw size, b is the location parameter and v is the scale parameter (Attachment I, DIRS 1, Sec. 6.2.1) (see DTN: MO9910SPAFWPWF.001 (Attachment I, DIRS 6)). Massari (Attachment I, DIRS 1, Sec. 6.2.1) states that all the references reviewed indicated that the PND for various size defects is dependent on a number of variables such as the type of material, operator skill, access to the weld, and type of defect. As all these factors cannot be determined at this point in time the parameters, b and v will be taken to be uncertain. Massari elicited values from the literature for b and v that range from 1.6 to 5-mm and 1 to 3 respectively. Therefore the probability that a flaw is not detected (let B be the set of flaws not detected) is then the definite integral from zero to the thickness of the weld:

$$Pr(B \mid b,v) = \int_0^t PND(s) \cdot f(s) \cdot ds .$$

The probability values to this integral for a 25-mm thick closure weld for various values for b and v are shown in Figure 1.

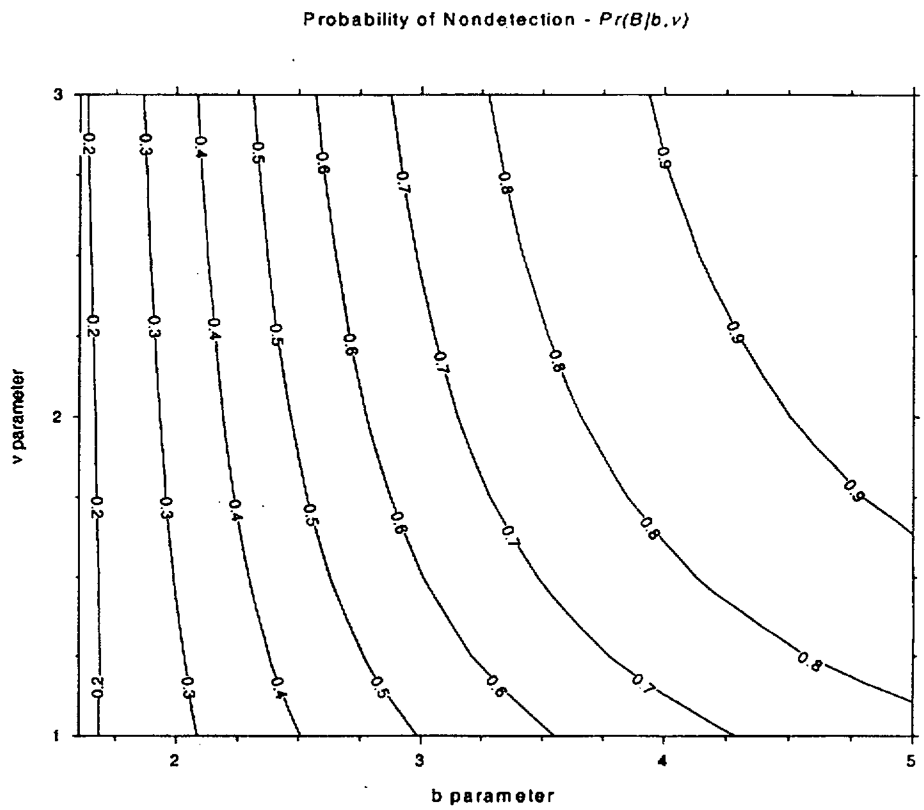


Figure 1. The probability flaws are not detected as a function of b and v (25-mm closure weld).

The conditional probability density function (pdf) for flaw size, s, (given that the flaw is not detected) is then:

$$g(s \mid b,v) = \frac{PND(s) \cdot f(s)}{Pr(B \mid b,v)}$$

Figure 2 shows several pdfs for a 25-mm thick closure weld for various combinations of values for b and ν.

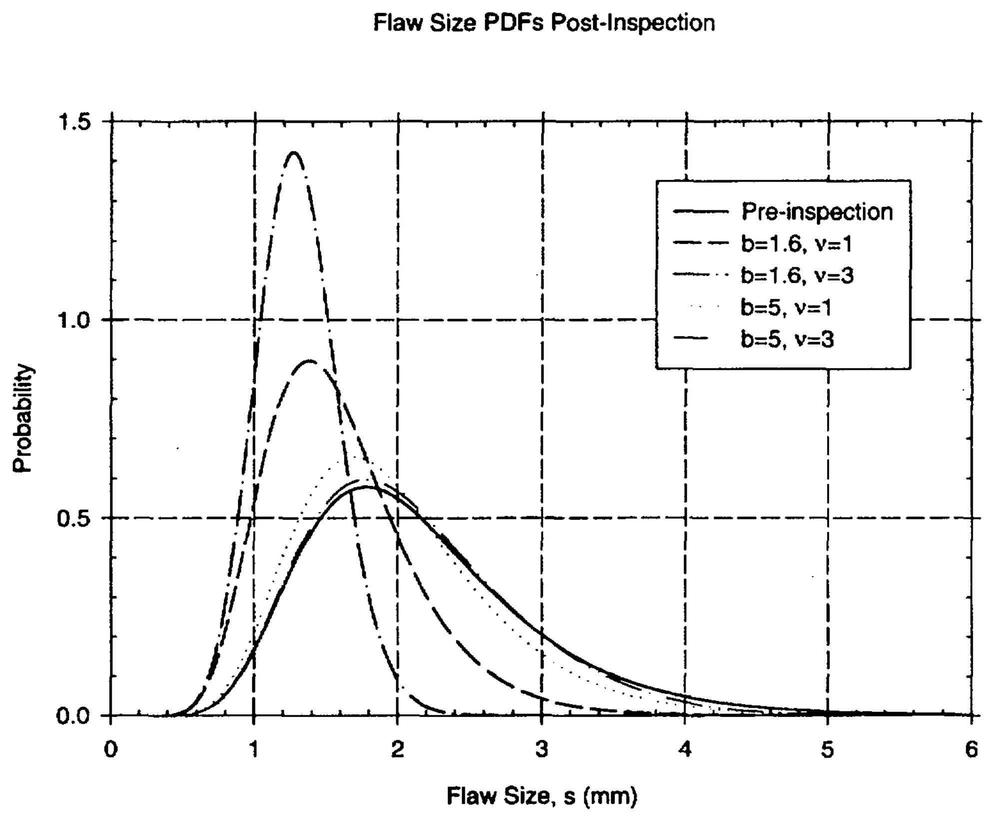


Figure 2. Conditional Probability Density Functions of Flaw Sizes (25-mm closure weld).

With cumulative distribution function given as,

$$G(s \mid b,\nu) = \frac{\int_0^s PND(x) \cdot f(x) \cdot dx}{Pr(B \mid b,\nu)}.$$

For weld thickness equal to 25mm and closure lid radius equal to 0.76 meters (DTN: MO9910SPAFWPWF.001), the mean flaw density of surface breaking flaws per closure weld, λ, may be given as function of the fraction of thickness, t, and surface breaking flaws, Ψ adjusted for the PND (given b and •) for the remaining flaws.

$$\lambda(t,\Psi,b,\nu) = 3.2658 \cdot [12.8 + 31.4 \cdot \Psi] \cdot R(t) \cdot \Psi \cdot \Pr(B \mid b,\nu)$$

The distribution of flaw occurrences on the closure weld of the waste package is modeled as a Poisson process.

Poisson Process Distribution

It is assumed that the number of flaws along a closure weld is Poisson distributed (Assumption 3.3). As a result, flaw occurrences in the weld are defined by the following five (Poisson process) properties:

1. There are no flaws at zero weld length. This amounts to an initial condition for the model.
2. The numbers of flaws that occur in nonoverlapping lengths of weld metal are independent.
3. The distribution of the number of flaws depends only on the length of weld metal considered.
4. For small weld segments, the probability of a flaw is proportional to the length of the weld. This constant of proportionality is denoted by λ.
5. There are no simultaneous flaws. This says that that the probability of obtaining two or more flaws in a sufficiently small segment of weld is negligible.

None of the assumptions above are unreasonable for modeling the stochastic occurrence of flaws given the generic welding process being considered (Attachment I, DIRS 5).

The Poisson parameter, λ, is the average value of the number of flaws/interval observed over many weld length intervals of the same size. The probability distribution of the number of flaws, X, for an interval of weld length, L, i.e., the Poisson distribution for the flaw density is given by

$$P(X = x) = \frac{(\lambda L)^x}{x!} exp(-\lambda L)$$

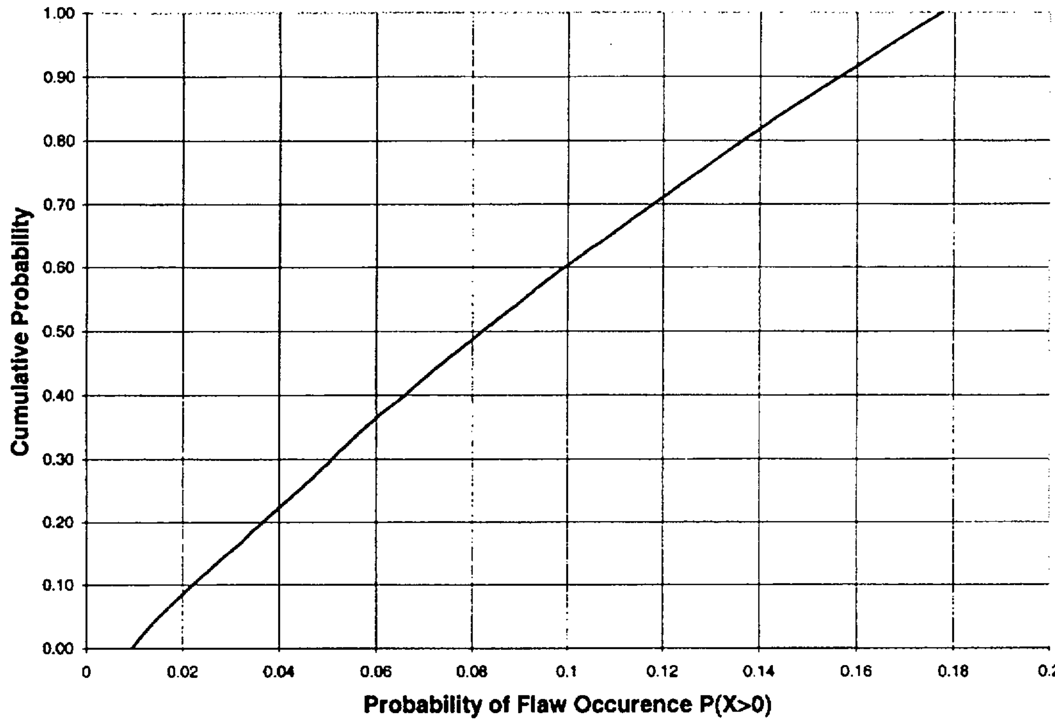
The probability of occurrence of flaws on a patch

$$P(X \geq 1) = 1 - P(X = 0) = 1 - exp(-\lambda L)$$

As given above, λ equals the mean flaw density for the number of flaws per closure weld. If there are N patches on a waste package, L could equal one divided by N.

Note that the flaw occurrence cdf for a patch depends on L, the length of weld that a patch weld would represent.

To illustrate the calculated range for the probability of the occurrence of flaws for a 25 mm lid, a cumulative density function (CDF) from a Monte Carlo simulation using the MFD DLL for ten thousand realizations is shown in Figure 3.



NOTE: CDF to illustrate the calculation results for Monte Carlo realizations using MFD code.

Figure 3. Probability of one or more flaws occuring on a 25-mm closure lid

6. RESULTS

Implementation of the calculation steps is described as follows. The number of flaws that appear on a patch is sampled stochastically as a Poisson random variable. For each flaw that occurs (i.e. when the number of flaws is not equal to zero) a flaw size is randomly assigned to it by sampling from the calculated flaw size cumulative distribution function $G(s)$. This flaw (for sampled location and size) is then used in the SCC analysis. The abstracted results are used as input to analyze its effect on waste package performance.

The main approach made in this abstraction is that, as these distributions treat the variability observed in flaws occurrence and size, some of the parameters that determine these distributions may need to be treated as uncertain. The instances of where uncertainty is included are for the parameters of 1) the flaw detection distributions (b and ν) and 2) the fraction of surface breaking flaws (Ψ). The parameters should be treated as follows.

The b and ν parameters of the detection distribution should be allowed to uniformly range between 1.6 to 5 mm and 1 to 3, respectively.

The fraction of surface breaking flaws, Ψ, in Massari's AMR (Attachment I, DIRS 1) (see DTN: MO9910SPAFWPWF.001 (Attachment I, DIRS 6)) is an average of three observations (average

(0.49%, 0.40%, 0.13%) = 0.34%). Instead of using a single value (i.e. 0.34%) it should be allowed to uniformly range from 0.13% to 0.49%.

The parameters should be varied independently. The planned sensitivity analysis with the proposed distributions of the parameters is to analyze the affect of not knowing the correct (deterministic) value of the parameters.

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

7. ATTACHMENTS

Attachment	Title
I	Document Input Reference System.
II	Mathcad Sheet - Probability and Size of Defect Flaws
III	MFD Software Routine Report

ATTACHMENT I

DOCUMENT INPUT REFERENCE SYSTEM

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

DOCUMENT INPUT REFERENCE SYSTEM

1. Document Identifier No./Rev.:	Change:	Title:
CAL-EBS-PA-000003 Rev. 00	N/A	CALCULATION OF PROBABILITY AND SIZE OF DEFECT FLAWS IN WASTE PACKAGE CLOSURE WELDS TO SUPPORT WAPDEG ANALYSIS

Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBVDue To		
2a.	2. Technical Product Input Source Title and Identifier(s) with Version	3. Section					Unqual.	From Uncontrolled Source	Un-Confirmed
1	CRWMS M&O 1999. *Analysis of Mechanisms for Early Waste Package Failure.* ANL-EBS-MD-000023 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19991101.0207.	6.2	N/A - Technical Product Output	Entire	Analysis of manufacturing defects.	N/A	N/A	N/A	N/A
2	CRWMS M&O 1999. *Calculations to Support WAPDEG Analysis of Waste Package and Drip Shield Degradation.* TDP-EBS-PA-000001 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990922.0220.	Entire	N/A - Reference Only	N/A	Technical Development Plan	N/A	N/A	N/A	N/A
3	CRWMS M&O 1999. *Stress Corrosion Cracking - Clarification on Analysis/Model Report.* Input Transmittal PA-WP-99317.Ta. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19991027.0158.	Attachment 1	N/A - Reference Only	N/A	Analysis of failure modes for stress corrosion cracking.	N/A	N/A	N/A	N/A
4	CRWMS M&O 1999. *Testing of Software Routine to Determine Deviate and Cumulative Probability: ModStandardNormal Version 1.0.* CAL-EBS-MD-000004 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19991018.0213.	Entire	N/A - Reference Only	N/A	Description of ModStandardNormal	N/A	N/A	N/A	N/A
5	Larson, H. J. 1982. *Introduction to Probability Theory and Statistical Inference.* New York, New York: John Wiley & Sons. TIC: 237892.	4.4	N/A - Reference Only	N/A	Discussion of Poisson Process	N/A	N/A	N/A	N/A
6	MO9910SPAFWPWF.001. Weld Flaws of Waste Packages. Submittal date: 10/22/1999.	Entire	N/A - Technical Product Output	Entire	Frequencies, size distributions, and orientations of waste package weld flaws.	N/A	N/A	N/A	N/A
7	Press, W.H.; Teukolsky, S.A.; Vetterling, W.T.; and Flannery, B.P. 1992. *Numerical Recipes in Fortran 77, The Art of Scientific Computing.* Volume 1 of *Fortran Numerical Recipes.* 2nd edition. Cambridge, United Kingdom: Cambridge University Press. TIC: 243606.	4.3	N/A - Reference Only	N/A	Use of Romberg integration	N/A	N/A	N/A	N/A

Attachment II
Mathcad Sheet - Probability and Size of Defect Flaws

$\text{thickness} := 10$

$p_{detection} := 0.005$

$$a_{50}(t) := \left(0.1159\cdot 25.4 - 0.0445\cdot t + \frac{0.00797}{25.4}\cdot t^2\right)$$

Geometric Mean of the Distribution

$$\sigma(t) := 0.09733 + \frac{0.3425}{25.4}\cdot t - \frac{0.07288}{25.4^2}\cdot t^2$$

Standard Deviation of the Distributi

$$\mu(t) := \ln(a_{50}(t))$$

$a_{50}(10) = 2.530238$ $\quad$ $a_{50}(25) = 2.027472$

$\sigma(10) = 0.220876$ $\quad$ $\sigma(25) = 0.363834$

$$A(s,b,v) := \left[\frac{(p_{detection} + 1)}{2} + \frac{(p_{detection} - 1)}{2}\cdot \text{erf}\left(v\cdot \ln\left(\frac{s}{b}\right)\right)\right]^2$$

$$f(s) := \frac{\exp\left[\frac{-\left(\ln\left(\frac{s}{a_{50}(\text{thickness})}\right)\right)^2}{2\cdot\sigma(\text{thickness})^2}\right]}{\sqrt{2\cdot\pi}\cdot\sigma(\text{thickness})\cdot s}$$

Log normal density function for the initial flaw size distribution

$$P_{ND}(b,v) := \int_0^{\text{thickness}} A(s,b,v)\cdot f(s)\,ds$$

Probability of non-detection Post Inspection

$$g(s,b,v) := \left| \begin{array}{l} D \leftarrow P_{ND}(b,v) \\ \dfrac{\overrightarrow{(A(s,b,v)\cdot f(s))}}{D} \end{array} \right.$$

The conditional probability density function for flaw size given flaw not detected

$$M1 := 8$$

$$M2 := 17$$

$$j := 0..M1$$

$$k := 0..M2$$

$$B_{j,k} := 1 + (3 - 1)\cdot\frac{j}{M1}$$

$$C_{j,k} := 1.6 + (5 - 1.6)\cdot\frac{k}{M2}$$

$$D_{j,k} := P_{ND}(C_{j,k}, B_{j,k})$$

$$M0 := (M1 + 1)\cdot(M2 + 1)$$

$$loc := 0..M0 - 1$$

$$B0_{loc} := B_{floor\left(\frac{loc}{M2+1}\right),\, loc-\left(floor\left(\frac{loc}{M2+1}\right)\right)\cdot(M2+1)}$$

$$C0_{loc} := C_{floor\left(\frac{loc}{M2+1}\right),\, loc-\left(floor\left(\frac{loc}{M2+1}\right)\right)\cdot(M2+1)}$$

$$D0_{loc} := D_{floor\left(\frac{loc}{M2+1}\right),\, loc-\left(floor\left(\frac{loc}{M2+1}\right)\right)\cdot(M2+1)}$$

$P_{ND}(1.6, 1) = 0.084$

$P_{ND}(1.6, 3) = 0.022$

$P_{ND}(2.5, 1) = 0.26$

$P_{ND}(5, 1) = 0.682$

$P_{ND}(5, 3) = 0.968$

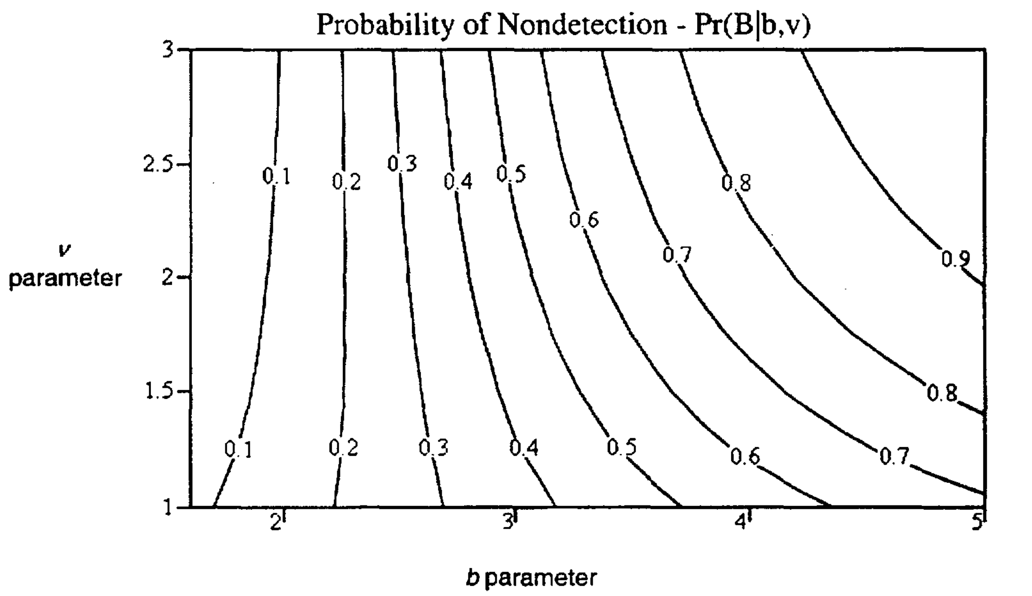


Figure 4. The probability flaws are not detected as a function of *b* and *v* (10-mm closure weld).

$N := 100$

$i := 0..N$

$n_i := \frac{i+1}{N+1}$

$d := 6 \cdot n$

$C0 := \overrightarrow{f(d)}$

$C1 := g(d, 1.6, 1)$

$C2 := g(d, 1.6, 3)$

$C3 := g(d, 5, 1)$

$C4 := g(d, 5, 3)$

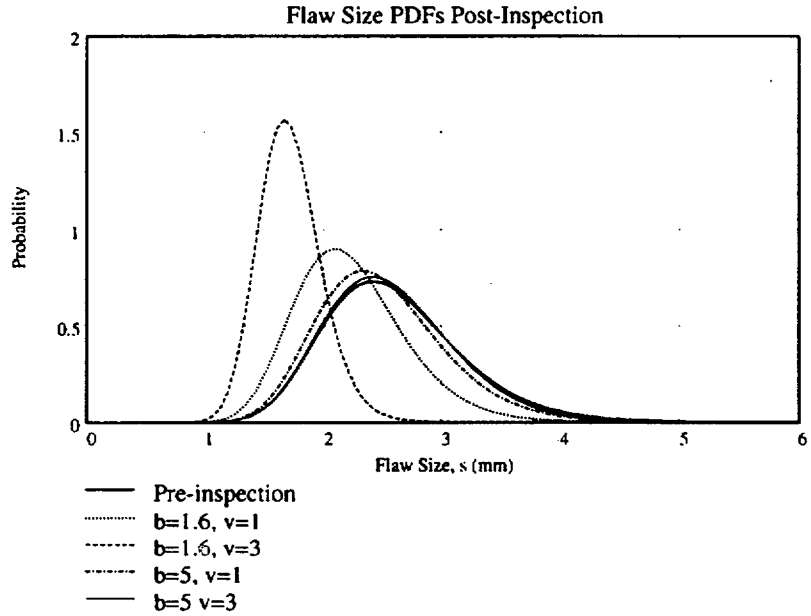


Figure 5. Conditional Probability Density Functions of Flaw Sizes (10-mm closure weld).

ATTACHMENT III

MFD SOFTWARE ROUTINE REPORT

1. SOFTWARE ROUTINE IDENTIFICATION

Name and Version Number - MFD (ManuFacturing Defects), version 1.01

This routine was developed using Microsoft Developer Studio 97 with Visual Fortran 5.0, Standard Edition.

SRR Document Identification Number: N/A

SRR Media Number (if applicable): N/A

2. DESCRIPTION AND TESTING

The software routine MFD calculates the cumulative probability distribution for the occurrence and size of manufacturing defects in the closure weld of waste packages given the non-detection probability and the fraction of surface breaking flaws. These calculations are based on the abstraction of flaw density and size distribution discussed in the body of this document. The outputs of MFD are:

A text file containing the cumulative distribution function (CDF) table for the number cracks (given that one or more cracks have occurred),
A text file containing the CDF table for crack sizes, and
An output argument containing the probability of at least one crack occurring.

2.1 DESCRIPTION OF SOFTWARE ROUTINE AND THE EXECUTION ENVIRONMENT

The MFD source code is a Fortran program 373 lines in extent. It conforms to the Fortran 90 standard and is thus highly portable. MFD was developed and tested in the Windows NT 4.0 operating system, and has been compiled with Visual Fortran 5.0, Standard Edition for Microsoft Windows 32 bit operating system environments. MFD may compile as a dynamic link library (MFD.DLL) which may be coupled with computer codes through external element mechanisms. MFD directly links and runs to simulate randomly occurring manufacturing defects for modeling waste package failures. The outputs are used by other Total System Performance codes to generate distributions for waste package failures.

The CDF file formats consists of a first line containing the number of rows in the CDF lookup table with the following lines containing two columns of numbers. The first column of numbers is the distribution values in increasing order. The second column contains the cumulative probability values.

Compilation of MFD requires several Fortran modules to be present from the WAPDEG library (CRWMS M&O 1999). These are modDefaultSize and modStandardNormal.

The bulk of MFD's coding is devoted to computing the cumulative probability of a manufacturing defect conditional to (based on) the probability for the non-detection of weld flaws. The parameters b and v define the probability for non-detection. This calculation also requires ψ the fraction of surface breaking fractures (Section 5). The inputs are read as part of the argument list of MFD, as the elements of array in(*):

in(1) = closure lid (weld) thickness (mm)
in(2) = closure lid radius (m)
in(3) = b, the location parameter of the non-detection probability
in(4) = v, the scale parameter of the non-detection probability
in(5) = ψ, the fraction of surface breaking fractures
in(6) = file index for the output file for CDF for the number of cracks
in(7) = file index for the output file for CDF for the size of cracks

The last two inputs are indices (line numbers) within a reference list file (WD4DLL.WAP) for filenames used by several DLLs (MFD being one) for waste package simulation.

The output consists of the CDFs written to the files indexed in(6) and in(7), and the probability of at least one crack per waste package (written to out(1)). The MFD DLL follows a project-coding standard that requires all DLL's to accept as input a method variable that controls the operation of the program. If a DLL is called with the following values of method, the following will occur:

method = 0	Initialize (MFD requires no initialization, thus nothing happens).
method = 1	Normal calculation (for MFD, compute the CDFs and probability of at least one crack occurring).
method = 2	Report the version number as out(1).
method = 3	Report the number of input and output arguments as out(1) and out(2), respectively (for MFD, this should yield the values 7 and 1, respectively).
method = 99	Clean up, close any open files.

2.2 DESCRIPTION OF THE ALGORITHM

MFD receives the input parameters from the argument list, and then follows the algorithm presented in the body of this document Section 6. Specifically, the following steps are performed:

1. Compute the conditional probability that the flaw is not detected, $\Pr(B \mid b, v)$. This is done numerically, via Rhomberg integration (Press, William H. et al. 1992. *Numerical Recipes in Fortran The Art of Scientific Computing Second Edition*. Cambridge, MA: Cambridge University Press. TIC: 243606).
2. Calculate $\lambda(\psi, b, v)$, the Poisson parameter rate for the number of cracks per closure weld.
3. Calculate the probability of at least one or more cracks per closure weld, pass this to out(1).

4. Evaluate the conditional (given one or more cracks have occurred) CDF for the number of cracks as a Poisson process with parameter $\lambda(\psi, b, \nu)$. Write the result to the file specified through in(6).
5. Evaluate the CDF of crack sizes, $G(s \mid b, \nu)$, as the convolution of the probability of non-detection (PND) and the flaw size distribution, divided by $\Pr(B \mid b, \nu)$. This is done numerically, via Rhomberg integration (Press et. al., 1992). Write the result to the file specified through in(7).

2.3 DESCRIPTION OF TEST CASE

The testing approach involves comparing the results of executing MFD and comparing the results with the example calculations presented in Attachment II of this document. The specific test case is to calculate the CDFs and the probability of at least one crack, given $P_{ND}(5,3)$ and ψ = 0.0034. The output CDFs and probability should be a reasonable match to the numerical results for this case in Attachment II of this document.

Running the MFD as a DLL, the following values are inserted as data elements in the MFD input stream:

in(1) = 10	thck
in(2) = 0.76	r
in(3) = 5	b
in(4) = 3	v
in(5) = 0.0034	ψ
in(6) = 3	idxnum
in(7) = 4	idxsiz

The test case requires one input file, a text file WD4DLL.wap, which is a list of filenames to be read by MFD. A listing of WD4DLL.wap is provided in Section 3. The third and fourth lines are the names of files used by MFD for the output CDFs for the number of cracks and the size of cracks, respectively.

2.4 DESCRIPTION OF TEST RESULTS

Comparison of the test case output files with those in this document, Attachment II, confirm that the MFD gives the anticipated results. The results also indicate that the probability of at least one crack should be 0.13718317. The output CDFs and probability are in agreement.

2.5 RANGE OF INPUT PARAMETER VALUES OVER WHICH RESULTS WERE VERIFIED

The preceding test case evaluates MFD for a typical set of parameters as observed from the manufacturing data

The waste package lid / weld thickness, for 10 and 25 (mm).
The waste package lid radius, for 0.76 (m).
The location parameter of the non-detection probability, *b*: for values 1.6 to 5 (mm).

The shape parameter of the non-detection probability, v for values 1 to 3.
The fraction of surface breaking fractures, ψ for values 0.0013 to 0.0049.

2.6 IDENTIFICATION OF LIMITATIONS ON SOFTWARE ROUTINE OR VALIDITY

MFD will execute properly if the following ranges and types of parameter values are met:

The waste package lid / weld thickness, a real number in the range 6.35 to 12.7 (mm) or the range 19.05 to 25.4 (mm). Other thickness ranges are not supported at this time.
The waste package lid radius, a positive real number in meters.
The location parameter of the non-detection probability, b: a positive real number (mm)
The shape parameter of the non-detection probability, v: a positive real number
The fraction of surface breaking fractures, ψ: a positive real number in the range 0 to 1.0

3. SUPPORTING INFORMATION

3.1 DIRECTORY LISTING OF EXECUTABLES AND DATA FILES

```
03/16/00  12:49p  mfd.f
03/16/00  11:35a  mfd.dll
03/16/00  03:05p  mfdcall.f
03/16/00  03:05p  mfdcall.exe
03/16/00  03:07p  mfdcall.out
01/27/00  01:54p  WD4DLL.wap
03/16/00  03:07p  WDMFD1test.txt
03/16/00  03:07p  WDMFD2test.txt
```

3.2 COMPUTER LISTING OF SOURCE CODE

```
SUBROUTINE mfd(method, state, in, out)
!
!  Subroutine to calculate the cdfs for canister defect occurrence
!  and size. This subroutine performs the following functions:
!  1. Argument list:
!      thck   closure lid (weld) thickness
!      r      closure lid radius
!      b      Location parameter for PND (probability of
!             nondetection) function (Uniform random variable)
!      v      Shape parameter for PND distribution
!             (Uniform random variable)
!      psi    Fraction of Surface Breaking Flaws.
!             (Uniform random variable)
!      idxnum File index for output conditional CDF
!             of number of cracks per WP.
!      idxsiz File index for output CDF of crack sizes
!  2. Calculate/Output:
!      CDF of number of cracks per WP (to file: numcdf).
!      CDF of crack sizes (to file: sizcdf).
!      flaw probability of one or more cracks per WP (to out(1)).
!
!DEC$ ATTRIBUTES dllexport,c :: mfd
```

```
!DEC$ ATTRIBUTES ALIAS : "mfd" :: mfd
!DEC$ ATTRIBUTES value       :: method
!DEC$ ATTRIBUTES reference   :: state
!DEC$ ATTRIBUTES reference   :: in
!DEC$ ATTRIBUTES reference   :: out
      USE ModDefaultsize
      USE ModStandardNormal
      IMPLICIT NONE
      integer(IKind) :: method   ! input, tells mfd what to do
      integer(IKind) :: state    ! return, 0 = OK
      real(RKind)    :: in(*)    ! input arguments
      real(RKind)    :: out(*)   ! output arguments
      real(RKind), PARAMETER :: VERSION = 1.01
      integer(IKind), PARAMETER :: NUMIN = 7, NUMOUT = 1
      integer(IKind), PARAMETER :: NSIZE = 200
      real(RKind), PARAMETER :: PI = 3.141592653589793
      integer(IKind) :: outunit, errunit, idxnum, idxsiz
      character(LEN = 80) :: numcdf, sizcdf, line1
      integer(IKind) :: n, i
      real(RKind) :: thck, r, b, v, psi, PrBbv, Lpbv, PrSbv, GSbv
      real(RKind) :: up, eps0, p0, p, size, step1, med, sdev, rdctn
      real(RKind) :: cpr(NSIZE)
!
!**********************************************************************
!
      if (method .eq. 0) then        ! Initialize
        state = 0
        return
      elseif (method .eq. 2) then    ! Report code version
        out(1) = VERSION
        state = 0
        return
      elseif (method .eq. 3) then    ! Report number of arguments
        out(1) = NUMIN
        out(2) = NUMOUT
        state = 0
        return
      elseif (method .eq. 1) then    ! Calculate
        thck   = in(1)
        r      = in(2)
        b      = in(3)
        v      = in(4)
        psi    = in(5)
        idxnum = in(6)
        idxsiz = in(7)
!
!  Open the file list and find the I/O filenames
!
        outunit = nextfreeunit()
        open(unit = outunit, file = 'WD4DLL.WAP')
        n = max(idxnum, idxsiz)
        do i = 1, n
          read(outunit,*) line1
          if (i .eq. idxnum) numcdf  = line1
          if (i .eq. idxsiz) sizcdf  = line1
        end do
        close(unit = outunit)
```

```
!
!  Evaluate the conditional probability Pr(B|b,v)
!  up   = upper bound of integration
!  eps0 = lower bound of integration
!  LOOK OUT HERE, ADJUSTING BOUNDS
!
         up = 8.0
         eps0 = 1.0E-20
         med = 0.1159*25.4 + thck*(-0.0445 + thck*0.00797/25.4)
         sdev = 0.09733 + thck*(0.3425 - thck*0.07288/25.4)/25.4
         call qromb(eps0, up, b, v, med, sdev, PrBbv, state)
         if (state .eq. 1_IKind) then
           errunit = nextfreeunit()
           open(unit = errunit, file = 'mfderror.log')
           write(errunit,*) 'Failure of qromb, 93'
           close(unit = errunit)
           return
         end if
!
!  Calculate the Poisson parameter (Lpbv)
!
         if ((thck .ge. 19.05) .and. (thck .le.25.4)) then
           rdctn = (60*thck - 635)/889
         else if  ((thck .ge. 6.35) .and. (thck .le. 12.7)) then
           rdctn = (-218*thck + 5207)/2845
         else
           errunit = nextfreeunit()
           open(unit = errunit, file = 'mfderror.log')
           write(errunit,*) 'Thickness out of range, method = ',method
           close(unit = errunit)
           state = 1
           return
         end if
         Lpbv = 0.6839*(12.8 + 31.4*psi)*rdctn*(2*PI*r)*psi*PrBbv
!
!  Evaluate the cumulative conditional probability distribution
!  of crack occurrence as a cumulative Poisson distribution and
!  write to file (numcdf).
!
         p0 = exp(-1.0_RKind*Lpbv)
         out(1) = 1.0_RKind - p0
         n = 1
         p = p0*Lpbv
         cpr(1) = p
         do while ((p .gt. 1.0D-14) .and. (n .lt. NSIZE))
           n = n+1
           p = p*Lpbv/dble(n)
           cpr(n) = cpr(n-1) + p
         end do
         outunit = nextfreeunit()
         open(unit = outunit, file = numcdf)
         write(outunit,*) 2*n
         write(outunit,'(1x,I11,1x,f18.15)') 1, 0.0
         do i = 1, n-1
           write(outunit,*) i, cpr(i)/out(1)
           write(outunit,*) i+1, cpr(i)/out(1)
         end do
```

```
        write(outunit,*) n, cpr(n)/out(1)
        write(outunit,*)
        write(outunit,3330) VERSION
        write(outunit,3331) out(1)
        write(outunit,3338) ( i, in(i), i = 1, NUMIN )
        write(outunit,*)
 3330   format('! Output from mfd version ',F4.2)
 3331   format('! For probability of flaw =',F12.8)
 3338   format('! argument in(',I2,') = ',f12.5)
        close(unit = outunit)
!
!  Evaluate the cumulative probability distribution of
!  crack sizes, G(s|b,v) and write to file (sizcdf).
!
        size = 0.0
        step1 = up/NSIZE
        outunit = nextfreeunit()
        open(outunit, file = sizcdf)
        write(outunit,*) NSIZE
        do i = 1, NSIZE
          size = size + step1
          call qromb (eps0, size, b, v, med, sdev, PrSbv, state)
          if (state .eq. 1_IKind) then
            errunit = nextfreeunit()
            open(unit = errunit, file = 'mfderror.log')
            write(errunit,*) 'Failure of qromb, 155'
            close(errunit)
            close(outunit)
            return
          end if
          GSbv = PrSbv / PrBbv
          write(outunit,*) size, GSbv
        end do
        write(outunit,*)
        write(outunit,3330) VERSION
        write(outunit,3331) out(1)
        write(outunit,3338) ( i, in(i), i = 1, NUMIN )
        write(outunit,*)
        close(unit = outunit)
        state = 0
        return
      elseif (method .eq. 99) then   ! Shut-down
        close(unit = outunit)
        close(unit = errunit)
        state = 0
        return
      else
        errunit = nextfreeunit()
        open(unit = errunit, file = 'mfderror.log')
        write(errunit,*) 'mfd crashed, method = ',method
        close(unit = errunit)
        state = 1
        return
      end if                         ! end block for method
      CONTAINS     ! qromb, polint, trapzd, nextfreeunit
!
!*********************************************************************
```

```
!
      SUBROUTINE qromb(a, b, p1, p2, p3, p4, ss, state)
!
!  Numerical integration of function 'pndf' from a to b via
!  Rhomberg integration, as described in Numerical Recipes Section 4.3.
!  Calls: polint, trapzd
!
      USE ModDefaultsize
      real(RKind) :: a, b, p1, p2, p3, p4, ss
      integer(IKind) :: state
      integer(IKind), PARAMETER :: JMAX = 30, JMAXP = JMAX+1
      integer(IKind), PARAMETER :: K = 5, KM = K-1
      real(RKind), PARAMETER :: EPS = 1.0e-12
      integer(IKind) :: j
      real(RKind) :: dss, h(JMAXP), s(JMAXP)

      h(1) = 1.0
      do j = 1, JMAX
        call trapzd(a,b,p1,p2,p3,p4,s(j),j)
        if (j .ge. K) then
          call polint(h(j-KM),s(j-KM),K,0,ss,dss,state)
          if (state .eq. 1_IKind) return
          if (abs(dss) .le. EPS*abs(ss)) return
        endif
        s(j+1) = s(j)
        h(j+1) = 0.25*h(j)
      end do
      state = 1    ! too many steps in qromb.
      return
      END SUBROUTINE qromb
!
!*********************************************************************
!
      SUBROUTINE polint(xa, ya, n, x, y, dy, state)
!
!  Polynomial interpolation for y given arrays xa and ya
!  (each of size n).  See Numerical Recipes Section 3.1
!  Calls: None
!
      USE ModDefaultsize
      integer(IKind), PARAMETER :: NMAX = 10
      integer(IKind) :: n, x, state
      real(RKind) :: dy, y, xa(n), ya(n)
      integer(IKind) :: i, m, ns
      real(RKind) :: den, dif, dift, ho, hp, w, c(NMAX), d(NMAX)
c
      ns = 1
      dif = abs(x-xa(1))
      do i = 1, n
        dift = abs(x-xa(i))
        if (dift .lt. dif) then
          ns = i
          dif = dift
        endif
        c(i) = ya(i)
        d(i) = ya(i)
      end do
```

```
      y = ya(ns)
      ns = ns-1
      do m = 1, n-1
        do i = 1, n-m
          ho = xa(i)-x
          hp = xa(i+m)-x
          w = c(i+1)-d(i)
          den = ho-hp
          if (den .eq. 0.) then
            state = 1  ! failure in polint.
            return
          end if
          den = w/den
          d(i) = hp*den
          c(i) = ho*den
        end do
        if (2*ns .lt. n-m) then
          dy = c(ns+1)
        else
          dy = d(ns)
          ns = ns-1
        endif
        y = y+dy
      end do
      return
      END SUBROUTINE polint
!
!**********************************************************************
!
      SUBROUTINE trapzd(a,b,p1,p2,p3,p4,s,n)
!
!  Evaluates trapezoidal rule for function pndf from a to b.
!  See Numerical Recipes Section 4.2.
!  Calls:
!  pndf(indep.variable, parameter1, parameter2, parameter3, parameter4)
!
      USE ModDefaultsize
      integer(IKind) :: n
      real(RKind) :: a, b, p1, p2, p3, p4, s
      integer(IKind) :: it, j
      real(RKind) :: del, sum, tnm, x
!
      if (n .eq. 1) then
        s = 0.5*(b-a)*(pndf(a,p1,p2,p3,p4)+pndf(b,p1,p2,p3,p4))
      else
        it = 2**(n-2)
        tnm = it
        del = (b-a)/tnm
        x = a + 0.5*del
        sum = 0.
        do j = 1, it
          sum = sum + pndf(x,p1,p2,p3,p4)
          x = x + del
        end do
        s = 0.5*( s + (b-a)*sum/tnm )
      endif
      return
```

```
      END SUBROUTINE trapzd
!
!************************************************************************
!
      real(RKind) FUNCTION pndf(s,b,v,med,sdev)
!
!  Calculates the integrand PND(s).f(s) used in the
!  integral for the conditional probability Pr(B|b,v).
!  Uses Erf(), the error function, from ModStandardNormal.
!
!  Input:  s     crack size (mm)
!          b     location parameter of PND
!          v     shape parameter of PND
!          med   location parameter of f
!          sdev  shape parameter of f
!  Output: (function value)
!
      real(RKind), PARAMETER :: P=0.005, PI=3.141592653589793
      real(RKind) :: s, b, v, med, sdev
      real(RKind) :: pnd, f
!
      if (s .le. 0) then
        stop !crack length invalid
        return
      end if
!
!  Calculate PND(s) and f(s)
!
      pnd = ( (P+1.0)/2.0 + (P-1.0)*Erf(.true.,v*log(s/b) )/2.0)
     +     * ( (P+1.0)/2.0 + (P-1.0)*Erf(.true.,v*log(s/b) )/2.0)
      f = (log(s/med))*(log(s/med)) / (2.0*sdev*sdev)
      f = exp(-f) / (s*sdev*sqrt(2*PI))
      pndf = pnd*f
      return
      END FUNCTION pndf
!
!************************************************************************
!
      integer(IKind) FUNCTION nextfreeunit()
!
!  Find the smallest unit number not currently attached and in use.
!  Avoid units 5 and 6.
!  Input : (none)
!  Output: (function value)
!  Local : i, InUse
!
!  Local variables
!
      integer(IKind) :: i
      logical InUse
!
      InUse = .true.
      i = 0
      do while (InUse)
        i = i + 1
        if(i .ne. 5 .and. i .ne. 6) then
          inquire(i, opened = InUse)
```

```
        end if
      end do
      nextfreeunit = i
      RETURN
      END FUNCTION nextfreeunit
!
!***********************************************************************
!
      END SUBROUTINE mfd
```

3.3 COMPUTER LISTING OF SOURCE CODE FOR TEST CALLER

Text of file mfdcall.f

```
PROGRAM mfdcall
!
!  Driver to test DLL mfd
!
      IMPLICIT NONE
      integer, PARAMETER :: intkind=4, rlkind=8
      integer(intkind), PARAMETER :: MAXIN = 7, MAXOUT = 2
      integer(intkind)  :: state       ! return, 0 = OK
      real(rlkind)      :: in(MAXIN)   ! input arguments
      real(rlkind)      :: out(MAXOUT) ! output arguments
!
      INTERFACE
        SUBROUTINE mfd(method, state, in, out)
        !DEC$ ATTRIBUTES DLLIMPORT :: mfd
        !DEC$ ATTRIBUTES ALIAS : "mfd" :: mfd
        !DEC$ ATTRIBUTES value :: method
        !DEC$ ATTRIBUTES reference :: state
        !DEC$ ATTRIBUTES reference :: in
        !DEC$ ATTRIBUTES reference :: out
        integer, PARAMETER :: intkind = 4, rlkind = 8
        integer(intkind)  :: method
        integer(intkind)  :: state   ! return, 0 = OK
        real(rlkind)      :: in(*)   ! input arguments
        real(rlkind)      :: out(*)  ! output arguments
        END SUBROUTINE mfd
      END INTERFACE
!
!  Initialize and
!  Assign test values to in array
!
      open(12,file='mfdcall.out')
      state = 0
      in(1) = 10          ! thck
      in(2) = 0.76        ! r
      in(3) = 5           ! b
      in(4) = 3           ! v
      in(5) = 0.0034      ! fraction of flaws
      in(6) = 3           ! idxnum
      in(7) = 4           ! idxsiz
!
!  Call DLL with calling sequence for method = 2, 3, 0, 1, 99
!
```

```
      CALL mfd(2, state, in, out)
      write(12,*) 'method = 2 run'
      write(12,121) out(1)
 121  format(1x,'version number:',f5.2)

      CALL mfd(3, state, in, out)
      write(12,*) 'method = 3 run'
      write(12,122) out(1), out(2)
 122  format(1x,'number of input and output arguments:',2f5.1)

      CALL mfd(0, state, in, out)
      write(12,*) 'method = 0 run'

      CALL mfd(1, state, in, out)
      write(12,*) 'method = 1 run'
      write(12,*) 'probability of at least one crack occurring =',out(1)

      CALL mfd(99,state, in, out)
      write(12,*) 'method = 99 run'

      END PROGRAM mfdcall
```

3.4 COMPUTER LISTING OF TEST DATA INPUT AND OUTPUT

Input text file (WD4DLL.wap).

```
WDMFD1gsim.txt
WDMFD2gsim.txt
WDMFD1test.txt
WDMFD2test.txt
```

Output text file of caller (mfdcall.out).

```
method = 2 run
version number: 1.01
method = 3 run
number of input and output arguments:  7.0  1.0
method = 0 run
method = 1 run
probability of at least one crack occurring =  0.137183171223015
method = 99 run
```

Output CDF for the number of cracks (file: WDMFD1test.txt).

```
20
           1  0.000000000000000
           1  0.928037232675321
           2  0.928037232675321
           2  0.996504506467805
           3  0.996504506467805
           3  0.999872020482346
           4  0.999872020482346
           4  0.999996242063074
           5  0.999996242063074
           5  0.999999907912968
```

```
 6  0.999999907912968
 6  0.999999998064074
 7  0.999999998064074
 7  0.999999999964367
 8  0.999999999964367
 8  0.999999999999416
 9  0.999999999999416
 9  0.999999999999991
10  0.999999999999991
10   1.00000000000000

! Output from mfd version 1.01
! For probability of flaw =  0.13718317
! argument in( 1) =      10.00000
! argument in( 2) =       0.76000
! argument in( 3) =       5.00000
! argument in( 4) =       3.00000
! argument in( 5) =       0.00340
! argument in( 6) =       3.00000
! argument in( 7) =       4.00000
```

Output CDF for the crack size (file: WDMFD2test.txt).

```
        200
 4.000000000000000E-002  6.122514873113449E-079
 8.000000000000000E-002  2.075328338612312E-055
 0.120000000000000       1.277161357176911E-043
 0.160000000000000       3.869600351908593E-036
 0.200000000000000       7.699163815038370E-031
 0.240000000000000       7.747981450177105E-027
 0.280000000000000       1.107948715129825E-023
 0.320000000000000       4.059079696319943E-021
 0.360000000000000       5.490443441651299E-019
 0.400000000000000       3.488297111033730E-017
 0.440000000000000       1.229208276756130E-015
 0.480000000000000       2.706166806296714E-014
 0.520000000000000       4.064257809297995E-013
 0.560000000000000       4.450509757610495E-012
 0.600000000000000       3.741005359287602E-011
 0.640000000000000       2.513685027270116E-010
 0.680000000000000       1.394589155763339E-009
 0.720000000000000       6.558422864012984E-009
 0.760000000000000       2.671328726614129E-008
 0.800000000000000       9.593776334480947E-008
 0.840000000000000       3.083775706138229E-007
 0.880000000000000       8.984484440126560E-007
 0.920000000000000       2.398225321282131E-006
 0.960000000000000       5.919369519086295E-006
  1.00000000000000       1.361765368024870E-005
  1.04000000000000       2.940132588232341E-005
  1.08000000000000       5.993548921316788E-005
  1.12000000000000       1.159703286694620E-004
  1.16000000000000       2.139814228382318E-004
  1.20000000000000       3.780592782246839E-004
  1.24000000000000       6.419297335403709E-004
  1.28000000000000       1.050936195250956E-003
  1.32000000000000       1.663778182569343E-003
  1.36000000000000       2.553786020741825E-003
  1.40000000000000       3.809523058259494E-003
  1.44000000000000       5.534544714393358E-003
  1.48000000000000       7.846204143358305E-003
  1.52000000000000       1.087347023069049E-002
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4. REFERENCES

CRWMS M&O 1999. *Testing of Software Routine to Determine Deviate and Cumulative Probability: ModStandardNormal Version 1.0.* CAL-EBS-MD-000004 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19991018.0213.

Press, William H., Teukolsky, Saul A., Vetterling, William T., Flannery, Brian P. 1992. *Numerical Recipes in Fortran 77, The Art of Scientific Computing.* Volume 1 of *Fortran Numerical Recipes.* 2nd edition. Cambridge, United Kingdom: Cambridge University Press. TIC: 243606.

2.3 USE OF U.S. NUCLEAR REGULATORY COMMISSION TECHNICAL POSITIONS AND REGULATORY GUIDES, AND INDUSTRY STANDARDS

2.3.1 Nuclear Regulatory Commission Technical Positions and Regulatory Guides

The U.S. Department of Energy (DOE) has used Nuclear Regulatory Commission (NRC) Technical Positions (staff, generic, or branch) and Regulatory Guides to adapt NRC's accepted direction of a process, practice, methodology, standard, limit, condition, or design approach in the design of a repository. Guidance from these NRC regulatory guidance documents, when expressed as design criteria in Section 1 of System Description Documents (SDDs), is a part of the regulatory design bases for that system. Chapters 4, 5, 6, and 9 address, in detail, application of these documents to the design of the repository. [The DOE philosophy of attempting to comply or be consistent with regulatory guides is not yet fully developed. Text will be provided in the future regarding that philosophy and the levels of compliance.]

Tables 2.1 and 2.2 identify, in summary form, the NRC Regulatory Guides and Technical Positions that are used at the geologic repository and the extent to which they are used. [Staff technical positions that are not applied because they are outdated, drafts, or superseded have not yet been identified fully.]

2.3.2 Codes and Standards

The DOE addresses, as a part of the regulatory design bases identified in Section 1 of the SDDs, those industry codes and standards identified in regulatory guidance documents. Application of these codes and standards are addressed in Chapters 4, 5, 6, and 9 regarding design of the repository. Compliance with NRC-accepted codes and standards ensures that the Monitored Geologic Repository (MGR) design is consistent with established regulatory precedent where appropriate. The selection of industry codes and standards, on an individual structure, system, or component (SSC) basis, is performed through the preparation of a Compliance Program Guidance Package for the relevant system and is captured as design input in Section 1 of the SDD. Development of guidance packages and SDDs are controlled by design-controlling procedures (NLP-3-36 and NLP-3-33, respectively).

Codes and standards comprise methods or criteria in a particular area that are based on proven practices and are mutually agreed upon through an industry-consensus process. Codes and standards identified by the NRC as acceptable and partially acceptable are provided in NUREG/CR-5973 (NRC 1996b). Codes and standards developed for another type of facility (e.g., nuclear power plant), but deemed appropriate for the MGR, will be used for detailed design, fabrication, construction, operation, and testing of structures, systems, and components (SSCs) as determined through preparation of a Compliance Program Guidance Package for the relevant system and captured as design input in Section 1 of related SDDs.

[The Code of Record has not yet been identified for design and construction of the repository and waste packages.] Section 2.5 and 2.6 provide information on implementation of codes and standards for SSCs that are important to radiological safety and important to waste isolation.

2.3.3 NRC Key Technical Issue – Repository Design and Thermal-Mechanical Effects, Subissue 1, Design Control Process

The primary issue for the Repository Design and Thermal-Mechanical Effects (RDTME) Key Technical Issue (KTI) is the adequacy of design, construction, and operation of the geologic repository operations area to meet the preclosure and postclosure performance objectives, taking into consideration the long-term thermal-mechanical processes. This KTI, through the related Issue Resolution Status Report (IRSR) (NRC 1998), has been divided into four subissues. This section addresses Subissue 1 of that IRSR, *Design Control Process: Implementation of an effective design control process within the overall quality assurance program.*

The Quality Assurance (QA) requirements for the MGR are specified in 10 CFR 63 (see 64 FR 8640), Subpart G. The requirements are based on the criteria of Appendix B of 10 CFR 50 and are applied to activities such as site characterization and repository design, construction, operations, and closure. Appendix B includes 18 criteria that comprise an effective QA program. In the IRSR, the NRC states that the application of Criterion III for "design control" of repository SSCs are of particular interest.

In Revision 0 of the RDTME IRSR (NRC 1997), the NRC found that the design control process used by the DOE for the Exploratory Studies Facility (ESF) was acceptable. Revision 1 of the IRSR identified 12 acceptance criteria related to Subissue 1 for acceptability of the MGR design control process. This subissue is addressed in its entirety in this section.

Current status of this subissue is that (as a result of the Appendix 7 meeting and document review by the NRC staff conducted during the week of June 8, 1998) the NRC has concluded that the DOE is maintaining adequate oversight of the design control process. One area of concern was noted and is addressed below. The NRC intends to continue to monitor the DOE's program by conducting focused reviews of selected vertical slices of MGR design documents that have been prepared by the DOE.

Resolution of this subissue is supported by the DOE demonstration that appropriate acceptance criteria for the subissue have been addressed, as follows.

- Criterion 1. The applicable regulatory requirements are identified.

  Discussion. DOE procedures direct that requirements be identified during the development of design documents. Examples of these requirements are evident, for example, in the procedure for analyses and models (AP-3.10Q) and in the procedure for system description documents (NLP-3-33). As expressed in the IRSR, the NRC found satisfactory compliance with this criterion.

- Criterion 2. The design bases associated with the regulatory requirements are defined.

  Discussion. DOE procedures require identification of system design bases [as defined in 10 CFR 63.2 (see 64 FR 8640)] as part of Section 1, "Functions and Design Criteria," of System Description Documents. As expressed in the IRSR, the NRC found satisfactory compliance with this criterion. (Note: 10 CFR 63.2 defines design bases as " that information that identifies the specific functions to be performed by a structure, system, or component of a facility and the specific values or ranges of values chosen for controlling parameters as reference bounds for design...")

- Criterion 3. The regulatory (Criterion 1) and design bases (Criterion 2) requirements are appropriately translated into specifications, drawings, procedures, and instructions.

  Discussion. As discussed, procedures that govern development of design documents specify inclusion of regulatory requirements and design bases into those documents. As expressed in the IRSR, the NRC found satisfactory implementation of this criterion.

- Criterion 4. Appropriate quality standards are specified in the design documents.

  Discussion. DOE procedures that govern development of design documents require specification of QA requirements in those documents. Examples of this are the procedure governing development of system description documents (NLP-3-33) and the procedure governing development of analyses and models (AP-3.10Q). As expressed in the IRSR, the NRC found satisfactory implementation of this criterion.

- Criterion 5. Any deviations from the standards specified under Criterion 4 are controlled properly.

  Discussion. The DOE procedure *To Be Verified (TBV) and To Be Determined (TBD) Monitoring System* (NLP-3-15) controls the use of unverified or undetermined scientific data, design requirements, engineering data, or performance assessment data subject to the QA program. The procedure establishes an identifier to track the status of TBV/TBD within documents that impact the MGR. As expressed in the IRSR, the NRC found satisfactory implementation of this criterion.

- Criterion 6. Measures are established for the selection of materials, parts, equipment, and processes that are essential to functions of SSCs and are important to safety and waste containment and isolation.

  Discussion. The DOE procedure *Specifications* (QAP-3-8) controls the development of performance and procurement specifications for the MGR. This procedure establishes requirements for specifying items or services to be obtained from suppliers and for the identification of design and material requirements and constraints that apply to all items and services within the scope of the specification. Specification development includes identification of inputs (which may originate in system description documents), analyses, or other sources. As expressed in the IRSR, the NRC found satisfactory implementation of this criterion.

- Criterion 7. Design interfaces are identified, controlled, and appropriately coordinated among participating design organizations.

  Discussion. The DOE procedure *MGR Interface Control Documentation* (NLP-3-34) establishes instructions for the management of interfaces among the various Yucca Mountain Site Characterization Project (YMP) segments and subsystems as required in the *Configuration Management Plan* (YMP 1995). The *Configuration Management*

Plan further addresses interface requirements at other levels in the configuration item hierarchical structure. As expressed in the IRSR, the NRC found satisfactory implementation of this criterion.

- Criterion 8. Procedures are established for review, approval, release, distribution, and revision of documents involving design interfaces.

  Discussion. The DOE procedure *MGR Interface Control Documentation* (NLP-3-34) establishes instructions for the management of interfaces among the various YMP segments and subsystems. The procedure allows use of the same methodology to develop interface control documents with external organizations and between project segments and subsystems. A process similar to that specified in NLP-3-34 is being used for these interfaces until specific procedures are developed. Interfaces between subsystems internal to an MGR system do not require management by procedure. As expressed in the IRSR, the NRC posed no concerns regarding implementation of this criterion.

- Criterion 9. Measures are established for verifying or checking the accuracy of design calculations (e.g., performing design reviews using alternate or simplified computational methods).

  Discussion. The DOE procedure *Analyses and Models* (AP-3.10Q) establishes requirements for the review of analyses and calculations. The procedure addresses assignment of checkers and reviewers and cites criteria to be included in the checks and reviews. It also addresses the validation of models through alternative approaches. The DOE procedure *Design Verification* (QAP-3-2) establishes requirements and describes the process for performing design verification of design outputs. Part of that process addresses design verification by use of alternate calculations or other methods. As expressed in the IRSR, the NRC posed no concerns regarding implementation of this criterion.

- Criterion 10. If testing is employed for verification of design adequacy, the testing is conducted under the most adverse conditions anticipated.

  Discussion. The DOE procedure *Design Verification* (QAP-3-2) implements this concept by requiring the establishment of test conditions that demonstrate adequacy of performance under the most adverse design conditions.

- Criterion 11. Design verification is done by independent and qualified professionals who were not among those who participated in the original design efforts.

  Discussion. The DOE procedure *Analyses and Models* (AP-3.10Q) establishes requirements for the review of analyses and models. This procedure addresses assignment of checkers and reviewers and cites criteria to be included in checks and reviews. A Product Checking Group (PCG) implements the checking function of this procedure. Through this practice, independence is achieved that is beyond the basic requirements of the QA program. The PCG also implements the checking function associated with the design procedures governing specifications (QAP-3-8), drawings (QAP-3-10), and others. The DOE procedure for *Design Verification* (QAP-3-2) establishes requirements for persons performing the verification and establishes that these persons must be individuals other than those who performed the original design and must be qualified in accordance with a the QA program. As expressed in the IRSR, the NRC posed no concerns regarding implementation of this criterion.

- Criterion 12. In addition to being applied to the original design, the design control process also is applied to design and field changes, and the changes are documented properly.

  Discussion. The DOE procedure *Impact Reviews of Revisions of Documents and Field/Laboratory Data that Affect the MGDS Development Organization* (NLP-3-26) establishes requirements to perform impact reviews to assure that such revisions are evaluated to ensure consistency between these documents and design products. Impact reviews are performed when design input requirements change, and documents are changed based on the results of the review. The NRC expressed a concern regarding this criterion in the IRSR. The DOE performed an evaluation and shared the concern. [Note: Action has been initiated to assure that individuals involved in this type of activity were advised of the concern and of the events that led to it. An assessment has been initiated to identify the extent of the identified problem. Until the actions are completed, a complete description of a resolution cannot be developed.

[These tables will be filled in as information becomes available]

Table 2-1. NRC Regulatory Guides

Title	Date/Rev	Applicability Partial or Full	Cross-reference to LA Section	Comments
1.89 Environmental Qualification of Certain Electric Equipment Important to Safety for Nuclear Power Plants (NRC 1984)	**June 1984/01**	**Partial**	4.1.1 and 4.1.6	This regulatory guide provides design criteria for critical components comprising safety related systems that must be available to ensure the health and safety of the public.

Table 2-2. NRC Technical Positions

Title	Date/Rev	Applicability Partial or Full	Cross-reference to LA Section	Comments
NUREG-1323 Branch Technical Position on the Use of Expert Elicitation in the High-Level Radioactive Waste Program (NRC 1996a)	**December 1996/00**	**Full**	5.1.4.1	If used, expert elicitation is conducted in accordance with NUREG-1563 or other acceptable approaches.

2.3 References

Documents Cited

NRC 1984. *Environmental Qualification of Certain Electric Equipment Important to Safety for Nuclear power Plants.* Regulatory Guide 1.89. Rev 00. Washington D.C. U. S. Nuclear Regulatory Commission. TIC: 238593.

NRC 1996b. *Codes and Standards and Other Guidance Cited in Regulatory Documents.* NUREG/CR-5973 (PNL-8462). REV 03. Washington D.C. NRC. TIC: 23267.

NRC 1996a. *Branch Technical Position on the Use of Expert Elicitation in the High-Level Radioactive Waste Program.* NUREG-1563. REV 00. Washington D.C. U. S. Nuclear Regulatory Commission. TIC: 226832.

NRC 1997. *Issue Resolution Status Report Key Technical Issue: Repository Design and Thermal-Mechanical Effects.* Rev 00. Washington D.C. U. S. Nuclear Regulatory Commission. TIC: 241953.

NRC 1998. *Issue Resolution Status Report Key Technical Issue: Repository Design and Thermal-Mechanical Effects.* REV 01. Washington D.C. U. S. Nuclear Regulatory Commission. TIC: 241517

YMP 1995. *Configuration Management Plan.* Rev 0. Las Vegas, Nevada: U.S. Department of Energy. MOL.19960126.0220.

Codes, Standards, and Regulations

10 CFR 50. *Energy: Domestic Licensing of Production and Utilization Facilities.* TIC 238441.

64 FR (Federal Register) 8640. *Disposal of High-Level Radioactive Wastes in a Proposed Geologic Repository at Yucca Mountain, Nevada.* Proposed rule: 10 CFR 63. Washington, D.C.: National Archives and Records Administration. TIC: 242725.

Procedures

DOE Procedures

AP-3.10Q. *Analyses and Models.* (Rev 0)

M&O Procedures

NLP-3-15. *To Be Verified (TBV) and To Be Determined (TBD) Monitoring System.* (Rev 5)

NLP-3-26. *Impact Reviews of Revisions of Documents and Field/Laboratory Data that Affect the MGDS Development Organization.* (Rev 0)

NLP-3-33. *System Description Documents.* (Rev 3)

NLP-3-34. *MGR Interface Control Documentation.* (Rev 1)

NLP-3-36. *Development of Compliance Program Guidance Packages.* (Rev 1)

QAP-3-2. *Design Verification.* (Rev 7)

QAP-3-8. *Specifications.* (Rev 8)

QAP-3-10. *Engineering Drawings.* (Rev 8)

2.3 Acronym List

DOE	U.S. Department of Energy
ESF	Exploratory Studies Facility
IRSR	Issue Resolution Status Report
KTI	Key Technical Issue
MGR	Monitored Geologic Repository
NRC	Nuclear Regulatory Commission
PCG	Product Checking Group
QA	Quality Assurance
RDTME	Repository Design and Thermal-Mechanical Effects
SDD	System Description Document
SSC	structure, system, or component