OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

1. QA: QA

ANALYSIS/MODEL COVER SHEET

Complete Only Applicable Items

2. ☒ Analysis	Check all that apply	3. ☐ Model	Check all that apply
Type of Analysis	☐ Engineering ☒ Performance Assessment ☐ Scientific	Type of Model	☐ Conceptual Model ☐ Abstraction Model ☐ Mathematical Model ☐ System Model ☐ Process Model
Intended Use of Analysis	☐ Input to Calculation ☒ Input to another Analysis or Model ☐ Input to Technical Document ☐ Input to other Technical Products	Intended Use of Model	☐ Input to Calculation ☐ Input to another Model or Analysis ☐ Input to Technical Document ☐ Input to other Technical Products
Describe use:		Describe use:	
To be used in TSPA-SR to calculate dose.			

4. Title:
Abstraction of BDCF Distributions for Irrigation Periods

5. Document Identifier (including Rev. No. and Change No., if applicable):
ANL-NBS-MD-000007, Rev. 00

6. Total Attachments:

7. Attachment Numbers - No. of Pages in Each:
I-1, II-6

		Printed Name	Signature	Date
8.	Originator	Anthony J. Smith	[signature]	14 Apr 00
9.	Checker	Ron McCurley	W R Arthur for R. McCurley	4/14/00
10.	Lead/Supervisor	Anthony J. Smith	[signature]	14 Apr 00
11.	Responsible Manager	Jerry McNeish	Jerry A McNeish	4.14.00

12. Remarks:

INFORMATION COPY

LAS VEGAS DOCUMENT CONTROL

NM3507

OFFICE OF CIVILIAN RADIOACTIVE WASTE
MANAGEMENTANALYSIS/MODEL REVISION RECORD
Complete Only Applicable Items

2. Analysis or Model Title:

Abstraction of BDCF Distributions for Irrigation Periods

3. Document Identifier (including Rev. No. and Change No., if applicable):

ANL-NBS-MD-000007, Rev. 00

4. Revision/Change No.	5. Description of Revision/Change
Revision 00	Initial Issue

DISCLAIMER

This contractor document was prepared for the U.S. Department of Energy (DOE), but has not undergone programmatic, policy, or publication review, and is provided for information only. The document provides preliminary information that may change based on new information or analysis, and represents a conservative treatment of parameters and assumptions to be used specifically for Total System Performance Assessment analyses. The document is a preliminary lower level contractor document and is not intended for publication or wide distribution.

Although this document has undergone technical reviews at the contractor organization, it has not undergone a DOE policy review. Therefore, the views and opinions of authors expressed may not state or reflect those of the DOE. However, in the interest of the rapid transfer of information, we are providing this document for your information per your request.

CONTENTS

Page

1. PURPOSE 6

2. QUALITY ASSURANCE 6

3. COMPUTER SOFTWARE AND MODEL USAGE 7

4. INPUTS 7
   - 4.1 DATA AND PARAMETERS 7
     - 4.1.1 BDCF Abstraction Parameters 7
     - 4.1.2 Soil Erosion Data 9
     - 4.1.3 Surface Soil Thickness 9
   - 4.2 CRITERIA 10
   - 4.3 CODES AND STANDARDS 10

5. ASSUMPTIONS 11

6. ANALYSIS/MODEL 11
   - 6.1 A SIMPLE ABSTRACTION FOR GENII-S BDCF EVOLUTION OVER TIME 11
   - 6.2 INCORPORATION OF SOIL EROSION LOSS MECHANISM INTO BDCF EVOLUTION 13
     - 6.2.1 Overview For Incorporation Of Additional Loss Mechanism 13
     - 6.2.2 Soil Erosion Parameter λ 14
   - 6.3 ANALYSIS OF THE GENII-S DISTRIBUTION PARAMETERS 15
   - 6.4 RESULTS OF FITTING FOR BDCF MEAN VALUES 15
   - 6.5 INCORPORATING SOIL EROSION INTO THE FITTED PARAMETERS 16
   - 6.6 BUILD-UP EFFECT ON THE DISTRIBUTION STANDARD DEVIATION 17

7. CONCLUSIONS 17
   - 7.1 SUMMARY 18
   - 7.2 FINDINGS 18
   - 7.3 RECOMMENDATIONS FOR TSPA-SR 18

8. INPUTS AND REFERENCES 21
   - 8.1 DOCUMENTS CITED 21
   - 8.2 CODES, STANDARDS, REGULATIONS AND PROCEDURES 22
   - 8.3 SOURCE DATA, LISTED BY DATA TRACKING NUMBER 22
     - 8.3.1 Input Data 22
     - 8.3.2 Output Data 22

ATTACHMENTS 23

FIGURES

Figure 1. Comparison of GENII-S Predicted Values of the BDCF as a Function of Previous Irrigation Periods with Predicted Analytical Fit for ^{229}Th..... 16

TABLES

Page

Table 1. Input Data from Predecessor AMR for those Radionuclides where the lognormal Distribution was Appropriate 8

Table 2. Input Data from Predecessor AMR for ^{90}Sr where the Shifted lognormal Distribution was Appropriate 9

Table 3. Parameter Values Resulting in the Best Fit 15

Table 4. Lognormal Fitting Parameters Before And After Soil Erosion Is Taken Into Account. 17

Table 5. Percentage Increases in BDCFs due to Radionuclide Build-up in Soil with and without Soil Erosion 19

Table 6. Lognormal log parameters (i.e., of $ln(x)$) recommended for use TSPA-SR 20

Table 7. Lognormal Geometric Parameters (of x) recommended for use TSPA-SR 20

1. PURPOSE

The purpose of this analysis is to derive the abstractions for the time evolution of the Biosphere Dose Conversion Factors (BDCFs) due to radionuclide build-up effects in soil to be used in Total System Performance Assessment for Site Recommendation (TSPA-SR). One predecessor Analysis and Modeling Report (AMR) titled "*Distribution Fitting to the Stochastic BDCF Data*" (CRWMS M&O 2000a) identified a justifiable approximating distribution for the BDCFs over an appropriate period of irrigation. The data analyzed in this predecessor AMR were generated under the QA program as reported in CRWMS M&O 2000b by the GENII-S code (Leigh et al. 1993). Another predecessor AMR "Evaluate Soil/Radionuclide Removal by Erosion and Leaching" (CRWMS M&O 2000c). assessed the radionuclide removal from contaminated soil by erosion. The soil erosion mechanism is not considered in the GENII-S code. This analysis will incorporate soil loss into the time evolution of BDCFs after prolonged periods of irrigation.

The biosphere models and the associated internal calculations performed in the stochastic GENII-S code are the same as those performed in the deterministic GENII code reported by Napier (Napier, et al 1988). The calculations incorporate the build-up and removal of radionuclides in agricultural surface soil for several processes. The processes considered within GENII-S are the duration (years) of previous irrigation with contaminated water, harvest removal, radioactive decay, and leaching to deeper soil layer (Napier, et al; 1988. Volume 1 Section 4.6 *Soil Contamination Model*, p. 4.56).

The activities described in this report were conducted in accordance with the Work Package Direction and Planning Document for Assessment of *Abstraction of BDCF Distributions* (CRWMS M&O 1999a).

2. QUALITY ASSURANCE

The quality assurance (QA) program applies to the development of this analysis documentation. The information provided in this analysis will be used for evaluating the post-closure performance of the Monitored Geologic Repository (MGR) waste package and engineered barrier segment. The Performance Assessment Operations (PAO) responsible manager has evaluated the technical document development activity in accordance with QAP-2-0, *Conduct of Activities*. The QAP-2-0 activity evaluation (CRWMS M&O 1999b) has determined that the preparation and review of this technical document is subject to *Quality Assurance Requirements and Description* (DOE 2000) requirements. The activity evaluation (CRWMS M&O 1999b) remains in effect even though QAP-2-0, *Conduct of Activities*, has been superseded by AP-2.16Q, *Activity Evaluation*. The effort reported in this AMR was conducted and documented in accordance with AP-3.10Q, *Analyses and Models* and AP-3.15Q, *Managing Technical Product Inputs*. A work plan was developed, issued, and utilized in the preparation of this document (CRWMS M&O 1999a). Since the analysis does not involve any field activity, there is no determination of importance evaluation developed in accordance with NLP-2-0, *Determination of Importance Evaluations*. There are no permanent items addressed in this AMR, so it is not subject to QAP-2-3, *Classification of Permanent Items*.

An evaluation of the control of electronic management of data has been performed for this activity (per AP-SV.1Q), and it was concluded that current processes are adequate to ensure the accuracy, completeness, and security of the data used in this activity.

3. COMPUTER SOFTWARE AND MODEL USAGE

No models were used or developed in this analysis. The only software used was a commercially available spreadsheet (Microsoft® Excel 97 SR-2). This spreadsheet was used as an aid in calculation; no routines, macros, or other applications were developed and used. Use of this software is documented in this report in accordance with AP-SI.1Q, *Software Management*. The routine used is documented in Attachment II.

4. INPUTS

4.1 DATA AND PARAMETERS

The data used in this analysis were developed by Performance Assessment in support of the Biosphere effort for TSPA-SR. All data and information used were provided by two AMRs identified in the following sections.

4.1.1 BDCF Abstraction Parameters

The BDCF abstraction parameters were developed in *Distribution Fitting to the Stochastic BDCF Data* (CRWMS M&O 2000a.) The numerical data analyzed in this AMR were obtained from the Technical Data Management System (TDMS) by its associated Data Tracking Number DTN:MO0003SPASEA08.005. These numerical data are reproduced in Tables 1 and 2. These Tables also show the periods of previous irrigation used when generating the BDCF data. In the source AMR (CRWMS M&O 2000a), these defined statistical distributions were demonstrated to provide a statistically acceptable fit to the individual stochastic BDCF data sets that reflected the uncertainty in the parameters defining the critical group and reference biosphere (CRWMS M&O 2000b). Thus the data and parameters used herein, are therefore appropriate for the analysis to be undertaken and subsequently reported in this AMR.

Identified in CRWMS M&O 2000a, is that build-up is only significant (that is greater than 15%) for ^{90}Sr, ^{137}Cs, ^{229}Th, ^{243}Am, and ^{232}U. It was also shown that the lognormal distribution provides an acceptable fit for four of these radionuclides, ^{137}Cs, ^{229}Th, ^{243}Am, and ^{232}U, to the stochastic BDCFs generated by the GENII-S code (CRWMS M&O 2000b). The data for these radionuclides are given in Table 1. In the case of ^{90}Sr, the lognormal fit was unacceptable but the shifted lognormal was adequate. The ^{90}Sr fitting data are reproduced in Table 2.

Table 1. Input Data from Predecessor AMR for those Radionuclides where the lognormal Distribution was Appropriate

Radionuclide	Irrigation Period	Scale Factor	Lognormal Log Mean	Lognormal Log SD
	(years)		See Notes for Units	
^{243}Am	0	1.E-03	1.5196	0.1511
^{243}Am	511		1.7045	0.1317
^{243}Am	1138		1.8546	0.1351
^{243}Am	1947		1.9726	0.1523
^{243}Am	3084		2.0694	0.1684
^{243}Am	5031		2.1529	0.1819
^{137}Cs	0	1.E-05	2.1282	0.2389
^{137}Cs	8		2.3652	0.2272
^{137}Cs	18		2.5378	0.2143
^{137}Cs	30		2.6743	0.2048
^{137}Cs	48		2.8005	0.1980
^{137}Cs	78		2.9118	0.2014
^{229}Th	0	1.E-03	1.5077	0.1541
^{229}Th	858		1.9951	0.1688
^{229}Th	1910		2.3025	0.2195
^{229}Th	3269		2.5117	0.2456
^{229}Th	5179		2.6622	0.2696
^{229}Th	8448		2.7698	0.2802
^{232}U	0	1.E-03	0.5216	0.1486
^{232}U	9		0.5701	0.1434
^{232}U	21		0.6309	0.141
^{232}U	36		0.6718	0.1329
^{232}U	57		0.7126	0.1372
^{232}U	93		0.7433	0.1396

DTN:MO0003SPASEA08.005

NOTES: SD = Standard Deviation

The units of the lognormal distribution parameters are such that when the lognormal distribution is sampled and the resultant number is multiplied by the scaling factor, the resultant BDCF is in units of rem/year per pico-Curie/liter.

Table 2. Input Data from Predecessor AMR for ^{90}Sr where the Shifted lognormal Distribution was Appropriate

Radionuclide/ Irrigation period	Irrigation Period	Scale Factor	Distribution		
			Shifted lognormal		
			Shift (s)	Log Mean	Log SD
	(years)		See Notes for Units		
^{90}Sr	0	1.E-04	1.1846	-0.6045	0.5944
^{90}Sr	5		1.2529	-0.2547	0.7046
^{90}Sr	12		1.3470	-0.0768	0.8227
^{90}Sr	21		1.4100	0.0339	0.9122
^{90}Sr	33		1.4954	0.0639	0.9835
^{90}Sr	53		1.5248	0.1143	1.0065

DTN:MO0003SPASEA08.005

NOTES: s = shift (translation of axis)

SD = Standard Deviation

The units of the shifted lognormal distribution parameters are such that when the lognormal distribution is sampled, the shift value added, and the resultant number multiplied by the scaling factor, the resultant BDCF is in units of rem/year per pico-Curie/liter.

4.1.2 Soil Erosion Data

In the AMR tilted "*Evaluate Soil/Radionuclide Removal by Erosion and Leaching*" (CRWMS M&O 2000c), Section 7, Summary and Conclusions contains the following statement on erosion. "*The annual soil depth reduction estimates for the soils occurring within a 5-km radius about Lathrop Wells ranged from a low of 0.026 cm/yr for the Shamock series with a bulk density of 1.70 g/cm^3 to a high of 0.080 cm/yr for the Arizo, Commski, Sanwell, and Yermo soils with bulk densities of 1.40 g/cm^3. However, with the exception of the Shamock series, which is a moderately deep, gravelly fine sandy loam soil and therefore less resilient to soil erosion before experiencing a reduction in productivity, the calculated annual soil depth reduction rates are generally between 0.06 and 0.08 cm/yr. For the conservative bounding case, soil erosion was minimized to negligible levels (i.e., no surface soil erosion loss).*" For the purposes of this analysis, the lower bound of the calculated annual soil depth reduction (viz. 0.06 cm/year) will be used to include the effect of contaminated soil loss into the build-up due to prolonged irrigation periods. This datum was retrieved using DTN SN9912T0512299.002.

4.1.3 Surface Soil Thickness

To be consistent with the GENII-S parameters used to generate the BDCFs (CRWMS M&O 2000b) a surface soil thickness of 15 cm was used in this analysis. This parameter is in the package with DTN MO9911RIB00064.000 (Environmental Transport Parameter Values for Dose Assessment. Submittal date: 11/12/1999).

4.2 CRITERIA

This AMR was prepared to conform with DOE interim guidance (Dyer 1999) which directs the use specified Subpart/Sections of the proposed NRC high-level waste rule, 10 CFR Part 63 (64 FR 8640). Specified Subparts of this proposed rule that are particularly applicable to data include Subpart B, Section 15 (Site Characterization) and Subpart E, Section 114 (Requirements for Performance Assessment).

The U.S. Nuclear Regulatory Commission's (NRC's) Total System Performance Assessment and Integration (TSPA&I) Issue Resolution Status Report (IRSR) (NRC 1998) establishes generic technical acceptance criteria. These criteria are considered by the NRC staff to be essential to a defensible, transparent, and comprehensive assessment methodology for the repository system. These regulatory acceptance criteria address five fundamental elements of the Department of Energy (DOE) TSPA model for the Yucca Mountain site, namely:

1. Data and model justification (focusing on sufficiency of data to support the conceptual basis of the process model and abstractions)

2. Data uncertainty and verification (focusing on technical basis for bounding assumptions and statistical representations of uncertainties and parameter variabilities)

3. Model uncertainty (focusing on alternative conceptual models consistent with available site data)

4. Model verification (focusing on testing of model abstractions using detailed process-level models and empirical observations)

5. Integration (focusing on appropriate and consistent coupling of model abstractions).

Relevant to the topic of this AMR, elements (1) through (4) of the acceptance criteria were used to generate the abstraction for, first, soil build-up effects and, second, incorporate soil erosion into build-up effects. For each radionuclide, for which build-up effects are significant, this AMR reduces the set of six discrete BDCF distributions to a condensed empirical form. The process must preserve the integrity of the data (elements 1 & 4) while retaining the uncertainty inherent in the biosphere model/data (elements 2 & 3). The process conducted by this AMR (and its predecessor) is part of element (5) of the NRC acceptance criteria. This element applies to the synthesis of process-level models as discussed in the Biosphere PMRs and the abstraction conducted here that will be integrated into the TSPA-SR predictive code. The details of how this integration is implemented in the TSPA code will be addressed in the TSPA-SR.

4.3 CODES AND STANDARDS

There are no applicable codes or standards.

5. ASSUMPTIONS

It is assumed that the data feed as defined in section 4.1, accurately and acceptably reflects the reference biosphere and the receptor as defined (Dyer 1999). The data discussed in 4.1, transmitted, and used in this analysis were developed under AP-3.10Q, *Analyses and Models*, and are therefore considered reasonable for use.

In Section 6.1, the assumption is made that there is only one reservoir (a modeling compartment where radionuclides can accumulate over a period of many years) of importance in the GENII model. This reservoir is soil where adsorption can cause radionuclides to build-up in concentration over time from continuing irrigation with contaminated groundwater. The GENII manual (Napier et al 1988) does not provide any statements that contradict this assumption. The finding of this effort, reported in Section 6.4, indicate that this assumption is valid, and no further confirmation is required.

6. ANALYSIS/MODEL

To achieve the stated purpose of this AMR, two analysis steps are needed. The first is to derive an acceptable abstraction of the variation in BDCFs distributions over time consistent with the statistical BDCF distributions given in 4.1.1 that were derived from the GENII-S calculations. The resulting abstraction would only incorporate the radionuclide loss mechanisms of harvest, leaching, and decay as incorporated in GENII (Napier et al. 1988. p. 4.56). The second step is to incorporate the additional loss mechanism of soil erosion into the abstraction predicting the radionuclide build-up in soils.

6.1 A SIMPLE ABSTRACTION FOR GENII-S BDCF EVOLUTION OVER TIME

To assess the effect of soil build-up from continuing irrigation on dose, BDCFs were calculated in the effort reported in CRWMS M&O 2000b after six periods of previous irrigation. The mean and standard deviation parameters of the optimal lognormal distribution for each of these sets of data were data inputs to this AMR and are defined in 4.1.1 were given in Table 1.

A BDCF for prescribed conditions is the annual committed dose that the receptor would receive if there were unit concentration of the specific radionuclide in the groundwater. Although the assessment of the all pathway dose is not a trivial problem, some basic concepts can be introduced for the sake of this analysis. First for a given radionuclide and set of conditions the BDCF can be considered to have two components. The first z_0 is a component that is independent of time (i.e., of previous irrigation periods). The second $z(t)$ is the time varying component that is dependent upon the dynamics (input/output or gain/loss) in the "radionuclide reservoirs" present in the system under consideration.

$$BDCF(t) = z_0 + z(t) \qquad \text{(Eq. 1)}$$

Examples of z_0 are components of the BDCF due to ingestion of drinking water and the intake of the radionuclide that enters the food chain by contact of the irrigation water with the leaf system

of the edible crop. For $z(t)$, examples are external exposure to radiation from contaminated soil, inhalation of re-suspended soil particles, and the radionuclides taken up by edible crop through their root system. The three examples given above all have soil as the radionuclide reservoir. It should be remembered that other reservoirs could exist and that each could have it own characteristic dynamics.

Consider now a single reservoir; for the purposes of this analysis, this reservoir can be taken to be soil. If it is shown necessary, it would be a simple matter to incorporate multiple reservoirs.

If the concentration of a radionuclide in the reservoir (soil) at time t is $q(t)$ then by the conservation rule (the "increase" over a time period must equal "in" minus "out" over that same time period),

$$\frac{dq(t)}{dt} = I - \lambda q(t)$$

(Eq. 2)

where, I is the rate at which radionuclides are added (in this case the irrigation rate with contaminated water) and λ (= $\lambda_1 + \lambda_2 + \lambda_3$) is the total removal coefficient (for GENII-S this includes the leaching rate λ_1, radioactive decay λ_2, and crop removal λ_3).

This equation can be rearranged into a form that can readily be integrated.

$$\frac{-\lambda dq(t)}{I - \lambda q(t)} = -\lambda dt$$

(Eq. 3)

On the left-hand side, we have the derivative of the denominator appearing in the numerator, so this can be easily integrated to give,

$$\ln(I - \lambda q(t)) = -\lambda t + c$$

(Eq. 4)

where c is a constant of integration.

Rearranging this equation gives,

$$q(t) = \frac{I - de^{-\lambda t}}{\lambda}$$

(Eq. 5)

where d is the transformed constant of integration given by $d = e^c$

At time $t = 0$, $q(t) = 0$, so $d = I$, and

$$q(t) = \frac{I(1-e^{-\lambda t})}{\lambda}$$

(Eq. 6)

The time varying component of the BDCF, $z(t)$, is proportional to the level of contamination in the particular reservoir under consideration, $q(t)$.

Therefore, using k as the constant of proportionality, we can write

$$BDCF(t) = z_0 + \frac{kI(1-e^{-\lambda t})}{\lambda}$$

(Eq. 7)

In the accompanying Excel spreadsheet showing the actual calculations, the constants in the above equation have been defined as B, C, and D, such that,

$$BDCF(t) = C + DB(1-e^{-\frac{t}{B}})$$

(Eq. 8)

As expected, Eq. 8 has the functional form (i.e., a constant plus a time dependent term) as defined in Eq. 1. The intent in this AMR is to use the available Excel functions to determine the parameter values (B, C, and D) that best fit this equation to the optimized distributions of the GENII-S data. In using the above equation to fit the distribution parameters, it was assumed that there is only one reservoir of importance (i.e., the soil) in play within the GENII-S code. If this assumption is correct, it will be evident from the juxtaposition of the actual and predicted responses. If this assumption is not valid, a multiple reservoir model (two or more of the above functions) will have to be developed and used.

From the above equation, it is obvious (by setting t to be zero) that C in Eq. 8 is the BDCF with no prior irrigation. This is the same parameter as z_0 in Eq. 1 and is discussed in Section 6.1. In addition, it can be seen that $C+DB$ is the asymptotic BDCF value (the exponential terms approaches zero) after an infinitely long period of irrigation. (As t becomes infinitely large, the negative exponential term in the equation becomes infinitesimally small.)

6.2 INCORPORATION OF SOIL EROSION LOSS MECHANISM INTO BDCF EVOLUTION

6.2.1 Overview For Incorporation Of Additional Loss Mechanism

If the Eq. 8 has been demonstrated (by using the GENII-S data) to provide a reasonable predictive tool for the time evolution of the BDCFs with the irrigation period, additional loss mechanisms can be incorporated and the appropriate BDCFs generated. The rate of radionuclide

loss parameter (λ) for the mechanisms in the GENII-S code will have been determined by the fitting process. This parameter can be updated to incorporate addition loss mechanisms,

$$\lambda_{revised} = \lambda_{GENII\text{-}S} + \lambda_{new\ mechanism}. \qquad \text{(Eq 9)}$$

Once the new value of λ has been determined, the time evolution of the BDCFs with the additional loss mechanism can be generated.

6.2.2 Soil Erosion Parameter λ

From Section 4.1, the appropriate soil parameter values are defined. The first is the thickness of the soil layer considered appropriate for determination of the leaching factors, 15 cm (Section 4.1.3). The second is the lower limit (conservative) of annual soil loss estimate of 0.06 cm/year (Section 4.1.2).

This analysis discussed in 4.1.2 uses the same approximation for the distribution of radionuclides in soil as is used in GENII-S. This approximation is that the surface soil (i.e., topsoil) has a radionuclide distribution of radionuclides with depth that is constant over the (15 cm) rooting zone (Napier, et al 1988 section 4.6.2). For cultivated soil, this is justified by assuming plowing (roto-tilling for home gardens) to this depth provides this uniform mixing.

If the total concentration of a radionuclide in the 15 cm. top soil layer is x (Ci per m^2), then the rate of loss due (solely) to erosion is given by

$$\frac{dx}{dt} = -\frac{rx}{d} \qquad \text{(Eq. 10)}$$

where, t is time (years), r (m) is the annual thickness of soil lost by erosion, and d (m) is the thickness of the soil layer (0.15m).

Substituting the values defined for the variables in this equation gives,

$$\frac{dx}{dt} = -4 \times 10^{-3} x \qquad \text{(Eq. 11)}$$

The characteristic period (i.e., the time required for the concentration to decrease by a factor of *e*, the base of the natural logaritms) appropriate for this loss mechanism is the reciprocal of the coefficient of x. Thus, for Amargosa Valley soils this value is 250 years [(0.004 per year)$^{-1}$]. Note that as we took the lower limit of the rate of loss due to erosion, this time estimate is an upper limit. Reference to Table 1, shows that for ^{243}Am, ^{137}Cs, and ^{229}Th, this predicted soil erosion mechanism (characteristic time of 250 years) is significant when compared to the GENII-S predicted build-up times (thousands of years).

6.3 ANALYSIS OF THE GENII-S DISTRIBUTION PARAMETERS

The analysis was conducted using the Excel spreadsheet and some of its built-in functions. The spreadsheet file that was used as a template to perform the analysis on each radionuclide input data set is documented in Attachment II. This documentation complies with AP-SI.1Q. Attachment II provides computational details of the Excel spreadsheet named EXPONENTIAL FITTING ROUTINE V1_0.xls Version 1. This attachment identifies the equation in each cell and provides the user step by step instructions on how to make use of the template to generate the required results. The procedure was performed on the input data for each radionuclides (^{90}Sr, ^{137}Cs, ^{229}Th, ^{243}Am, and ^{232}U).

6.4 RESULTS OF FITTING FOR BDCF MEAN VALUES

The parameters determined to provide the optimum fit to the GENII-S data are provided in Table 2. The final row gives the largest fractional deviation

i.e., $MAX\left|\frac{(predicted - observed)}{predicted}\right|$ between the GENII-S distribution data and the fit as defined above for each of the radionuclides. As in all cases, the maximum absolute error is less than one percent, it is considered that the single reservoir approach is justified, with no need to attempt a higher order approximation.

Table 3. Parameter Values Resulting in the Best Fit

Parameter	RADIONUCLUDE				
	^{234}Am	^{137}Cs	^{90}Sr	^{229}Th	^{232}U
B	2231.621	40.23565	13.86008	3273.721	32.42595
C	4.576954	8.465581	1.73815	4.514005	1.67157
D	0.002013	0.287027	0.066192	0.003779	0.013689
Max Relative Deviation	0.28%	0.93%	0.60%	0.18%	0.79%

Figure 1 gives the graphical representation of the data points and fit for ^{229}Th, the radionuclide with the greatest build-up effect.

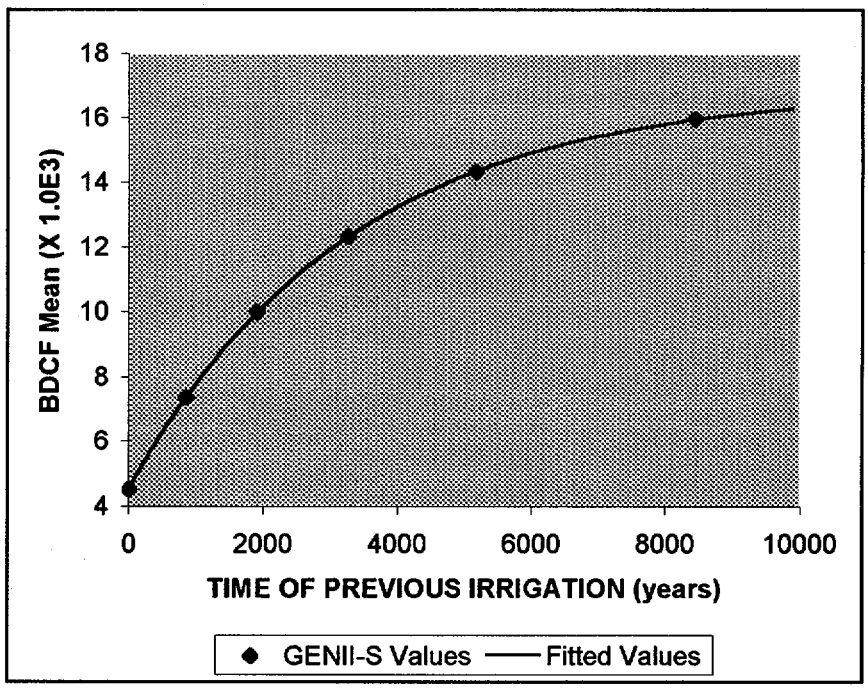

Figure 1. Comparison of GENII-S Predicted Values of the BDCF as a Function of Previous Irrigation Periods with Predicted Analytical Fit for ^{229}Th

6.5 INCORPORATING SOIL EROSION INTO THE FITTED PARAMETERS

The soil loss mechanism has its own characteristic loss rate (see 6.2.2.). As shown in 6.2.1, (Eq. 9) $\lambda_{new}=\lambda_{old} + \lambda_{soil\ loss}$. As from 6.1 $\lambda = 1/B$, then

$$B_{new}^{-1} = B_{old}^{-1} + B_{erosion}^{-1}$$

(Eq. 12)

This calculation is given in the attached spreadsheet in the Summary worksheet and reproduced in Table 3.

As indicated in Section 6.1, it is a trivial matter to determine the BDCF values appropriate for zero previous irrigation (C) and the asymptotic value after a long period of previous irrigation ($C + DB$). These values have been calculated and included in Table 4 for BDCFs with and without soil loss.

Table 4. Lognormal Fitting Parameters Before And After Soil Erosion Is Taken Into Account

Parameter	RADIONUCLUDE				
	^{243}Am	^{137}Cs	^{90}Sr	^{229}Th	^{232}U
B_{old}	2231.621	40.23565	13.86008	3273.721	32.42595
λ_{old}	4.48E-04	2.49E-02	7.21E-02	3.05E-04	3.08E-02
λ_{soil}	4.00E-03	4.00E-03	4.00E-03	4.00E-03	4.00E-03
λ_{new}	4.45E-03	2.89E-02	7.61E-02	4.31E-03	3.48E-02
B_{new}	224.815	34.658	13.132	232.263	28.703
C	4.576954	8.465581	1.73815	4.514005	1.67157
D	0.002013	0.287027	0.066192	0.003779	0.013689
Mean BDCF no previous Irrigation	4.577	8.466	1.738	4.514	1.672
Late Time Mean BDCF with no Erosion	9.070	20.014	2.656	16.884	2.115
Late Time Mean BDCF with Erosion	5.030	18.413	2.607	5.392	2.064
Build-up Factor no Erosion	1.98	2.36	1.53	3.74	1.27
Build-up Factor with Erosion	1.10	2.18	1.50	1.19	1.24

It is no surprise to find that soil loss, with its characteristic time scale of 250 years, has a dominant effect on the expected BDCF build-up for ^{229}Th, ^{137}Cs, and ^{243}Am where the GENII-S build-up periods are about two thousand years. Thus for these three radionuclides there is no need to consider the potential of previous irrigation much greater than a few hundred years. In fact, for these all five isotopes, the degree of build-up (up to 50 percent) is of no great significance and a recommendation will be made in Section 7, that the BDCF distribution associated with maximum build-up be used.

6.6 BUILD-UP EFFECT ON THE DISTRIBUTION STANDARD DEVIATION

Both linear and quadratic fitting functions for the standard deviations were considered. Neither gave the good degree of fit that was observed for the distribution means. However, when soil loss was considered (in Section 6.5) the build-up periods for ^{229}Th and ^{243}Am were much reduced (by about a factor of 10). The time scale over which build-up occurs for these radionuclides is the inverse of λ_{new} in Table 4. The times are 224 years for ^{243}Am and 232 years for ^{229}Th which, as expected, is a little less than the characteristic time used for soil removal (250 years). This time scale is closer to the values used to generate the BDCF data for period 1 (no previous irrigation). Therefore, it was considered reasonable to use the standard deviation values generated by GENII-S for period 1 (zero previous irrigation).

For ^{90}Sr and ^{232}U the GENII-S predicted build-up periods were sufficiently short that soil erosion could play any significant action of radionuclide removal. For these radionuclide it was considered conservative to ignore the erosion process and use the distributions and parameters applicable to the asymptotic BDCF value.

7. CONCLUSIONS

This document may be affected by technical product 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.

7.1 SUMMARY

Five radionuclides (^{90}Sr, ^{137}Cs, ^{229}Th, ^{243}Am, and ^{232}U) were identified in a predecessor AMR (CRWMS M&O 2000b) to have significant BDCF build-up factors from prior irrigation. Such an increase in BDCFs could have a significant impact on dose calculations in TSPA-SR for a community that has farmed the same land for many years. The distribution fitting used the raw BDCF information had been generated by the GENII-S. GENII-S does not consider soil erosion as a radionuclide loss mechanism. Soil loss was addressed in another predecessor AMR (CRWMS M&O 2000c).

The purpose of this AMR effort was twofold. First, to develop and fit an analytical approximation for the GENII-S generated build-up effect. Second, to incorporate into this approximation the soil loss data generated by CRWMS M&O 2000c. The result is to provide Performance Assessment with an abstraction for soil build up effects on BDCFs to be used to calculate dose.

7.2 FINDINGS

The approximation, developed using a mass balance equation, provided a good representation of the time evolution for the BDCF (lognormal distribution and shifted lognormal distribution) means as a function of irrigation times. For ^{229}Th and ^{243}Am, in the absence of soil loss, the time to approach the build-up limit was a few thousand years. Soil loss, with a predicted characteristic time constant of 250 years, has a significant effect on BDCF build-up for these three radionuclides. The effect soil erosion on ^{90}Sr, ^{137}Cs, and ^{232}U (with much shorter GENII-S build-up time of between 12 to 36 years) was, as expected, much less pronounced.

The degree of build-up for ^{229}Th and ^{243}Am, once soil loss was considered, was sufficiently small (less than 20 percent), that there was little benefit of incorporating a stochastic sampling for the time of previous irrigation. Rather, the conservative approach of using the asymptotic (i.e., long time) BDCF mean was used. The calculated standard deviation appropriate to time scale of interest (around 250 years) is recommended for sampling. The merits of this conservative approach were reinforced by the findings of Viability Assessment (DOE 1998, Volume 3, Figure 4-20 and 4-21). Here the study did not identify any of these radionuclides as being significant contributors to dose via the groundwater pathway at any time out to a million years.

For ^{90}Sr, ^{137}Cs, and ^{232}U, soil erosion had little effect of BDCFs. Again, the long time (period 6) value of the BDCF mean was used. The standard deviation calculated for the longest previous irrigation period. In the case of ^{90}Sr the shifted lognormal distribution was used.

7.3 RECOMMENDATIONS FOR TSPA-SR

The work reported in this AMR permits the following recommendations are made for TSPA-SR.

The soil loss mechanism is included in the BDCFs for the three radionuclides (^{229}Th, ^{243}Am, and ^{232}U) where the GENII-S predictions show a significant (greater than 15%) build-up in BDCF values from previous irrigation periods.

Due to the reduction in the degree of BDCF build-up from previous irrigation once soil erosion is considered, it is recommended that mean BDCF appropriate to the time-asymptotic values are used (see Table 4). The soil build-up factors without and with soil erosion are given in Table 5.

Table 5. Percentage Increases in BDCFs due to Radionuclide Build-up in Soil with and without Soil Erosion

Radionuclide	Increase in BDCF due to Soil Build-up	
	With No Soil Erosion	With Soil Erosion
^{229}Th	274%	19%
^{243}Am	98%	10%
^{232}U	27%	24%
^{137}Cs	136%	118%
^{90}Sr	53%	50%.

Because of the large decrease in the time scales associated with build-up when the soil erosion mechanism is taken into account, the standard deviation appropriate to the zero previous irrigation is used for ^{229}Th and ^{243}Am.

For ^{232}U the standard deviation of the lognormal fitted distribution shows only a small variability with irrigation period, it is recommended that the time zero standard deviation be used for BDCF sampling.

For ^{90}Sr the standard deviation of the shifted lognormal fitted distribution is recommended using the parameters derived for the longest period of irrigation.

The recommended lognormal parameters for the radionuclides with soil erosion included are given in Table 6. In the event, that the geometric parameters (*e* raised to the power of the appropriate parameter in Table 6) of the lognormal distribution are required these are given in Table 7.

To generate the stochastic BDCFs (in units of rem/year per picoCurie/liter) from the data given in Table 5, the following steps are taken.

(a) Use the TSPA code to randomly sample for a lognormal distribution with the defined (log) mean and (log) standard deviation.

(b) In the case of the shifted lognormal distribution add the offset to the value derived in (a).

(c) Multiply the resulting number by the scaling factor.

(d) The result is the BDCF for the specified radionuclide that reflects the uncertainty in the Biosphere Model.

Table 6. Lognormal log parameters (i.e., of *ln(x)*) recommended for use TSPA-SR

Parameter	RADIONUCLUDE ^{243}Am	^{229}Th	^{232}U	^{137}Cs	^{90}Sr
Scaling Factor	1.0E-03	1.0E-03	1.0E-03	1.0E-05	1.0E-04
Distribution	Lognormal	Lognormal	lognormal	Lognormal	Shifted lognormal
Shift	N/A	N/A	N/A	N/A	1.525
Mean	1.615	1.685	0.725	2.913	0.114
SD	0.151	0.154	0.140	0.151	1.006

NOTES: SD = Standard Deviation

The units of the lognormal distribution parameters are such that when the lognormal distribution is sampled and the resultant number is multiplied by the scaling factor, the resultant BDCF is in units of rem/year per pico-Curie/liter.

The units of the shifted lognormal distribution parameters are such that when the lognormal distribution is sampled, the shift value added, and the resultant number multiplied by the scaling factor, the resultant BDCF is in units of rem/year per pico-Curie/liter.

Table 7. Lognormal Geometric Parameters (of *x*) recommended for use TSPA-SR

Parameter	RADIONUCLUDE ^{243}Am	^{229}Th	^{232}U	^{137}Cs	^{90}Sr
Scaling Factor	1.0E-03	1.0E-03	1.0E-03	1.0E-05	1.0E-04
Distribution	Lognormal	Lognormal	lognormal	Lognormal	Shifted lognormal
Shift	N/A	N/A	N/A	N/A	1.525
Mean	5.030	5.392	2.064	18.413	1.121
SD	1.163	1.167	1.150	1.163	2.736

DTN:MO000SPAABS07.006

NOTES: SD = Standard Deviation

The units of the lognormal distribution parameters are such that when the lognormal distribution is sampled and the resultant number is multiplied by the scaling factor, the resultant BDCF is in units of rem/year per pico-Curie/liter.

The units of the shifted lognormal distribution parameters are such that when the lognormal distribution is sampled, the shift value added, and the resultant number multiplied by the scaling factor, the resultant BDCF is in units of rem/year per pico-Curie/liter.

8. INPUTS AND REFERENCES

8.1 DOCUMENTS CITED

CRWMS M&O (Civilian Radioactive Waste Management System Management and Operating Contractor) 1999a. *Abstraction of BDCF Distributions (Rev. 01), ID: F2000, Activity: SSPMR280.* Work Direction and Planning Document. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990707.0094.

CRWMS M&O 1999b. *Conduct of Performance Assessment.* Activity Evaluation, September 30, 1999. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19991028.0092.

CRWMS M&O 2000a. *Distribution Fitting to the Stochastic BDCF Data.* ANL-NBS-MD-000008 REV 00. Las Vegas, Nevada: CRWMS M&O. Submit to RPC URN-0140

CRWMS M&O 2000b. *Evaluate Soil/Radionuclide Removal by Erosion and Leaching.* ANL-NBS-MD-000009 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20000310.0057.

CRWMS M&O 2000c. *Non-Disruptive Event Biosphere Dose Conversion Factors.* ANL-MGR-MD-000009 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20000307.0383.

DOE (U.S. Department of Energy) 1998. *Total System Performance Assessment.* Volume 3 of *Viability Assessment of a Repository at Yucca Mountain.* DOE/RW-0508. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.19981007.0030.

DOE 2000. *Quality Assurance Requirements and Description.* DOE/RW-0333P, Rev. 9. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.19991028.0012.

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

Leigh, C.D.; Thompson, B.M.; Campbell, J.E.; Longsine, D.E.; Kennedy, R.A.; and Napier, B.A. 1993. *User's Guide for GENII-S: A Code for Statistical and Deterministic Simulations of Radiation Doses to Humans from Radionuclides in the Environment.* SAND91-0561. Albuquerque, New Mexico: Sandia National Laboratories. TIC: 231133.

Napier, B.A.; Peloquin, R.A.; Strenge, D.L.; and Ramsdell, J.V. 1988. *Conceptual Representation.* Volume 1 of *GENII: The Hanford Environmental Radiation Dosimetry Software System.* PNL-6584. Richland, Washington: Pacific Northwest Laboratory. TIC: 206898.

NRC (U.S. Nuclear Regulatory Commission) 1998. *Issue Resolution Status Report Key Technical Issue: Total System Performance Assessment and Integration.* Rev. 1. Washington, D.C.: U.S. Nuclear Regulatory Commission. ACC: MOL.19990105.0083.

8.2 CODES, STANDARDS, REGULATIONS AND PROCEDURES

AP-3.10Q, Rev.2, ICN 0. *Analyses and Models.* Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20000217.0246.

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

AP-2.16Q. *Activity Evaluation.* Washington, D.C.: DOE, OCRWM. ACC: MOL.20000207.0716.

AP-SI.1Q, Rev. 2, ICN 4. *Software Management.* Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20000223.0508.

NLP-2-0, Rev. 5. *Determination of Importance Evaluations.* Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.19981116.0120.

QAP-2-0, Rev. 5. Conduct of Activities. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980826.0209.

QAP-2-3, Rev. 10. *Classification of Permanent Items.* Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.19990316.0006.

8.3 SOURCE DATA, LISTED BY DATA TRACKING NUMBER

8.3.1 Input Data

MO0003SPASEA08.005. Abstracted BDCF Distributions for Use in Soil Erosion Analysis. Submittal date: 03/21/2000. Submit to RPC URN-0226

MO9911RIB00064.000. Environmental Transport Parameter Values for Dose Assessment. Submittal date: 11/10/1999.

SN9912T0512299.002. Annual Surface Soil Removal Estimates for Amargosa Valley Soils. Submittal date: 12/09/1999.

8.3.2 Output Data

MO0003SPAABS07.006. Abstracted BDCF Distribution with Soil Erosion for Use in TSPA-SR. Submittal date: 03/19/2000.

ATTACHMENTS

The attachments are listed as follows:

Attachment	Title
1	List of Acronyms
2	Spreadsheet Calculation To Optimize The Goodness Of Fit Of The Single Exponential Representation Of BDCF Abstractions Due To Radionuclide Build-Up In Soil As A Result Of Periods Of Previous Irrigation With Contaminated Groundwater (Exponential Fitting Template V1_0 with File name EXPONENTIAL FITTING ROUTINE V1_0.XLS Version 1.0)

ATTACHMENT 1

LIST OF ACRONYMS AND ABBREVIATIONS

AMR	Analysis/Modeling Report
BDCF	Biosphere Dose Conversion Factor
CRWMS M&O	Civilian Radioactive Waste Management Systems Management and Operating Contractor
DOE	Department of Energy
IRSR	Issue Resolution Status Report
MAX	Maximum (Excel function)
NRC	US Nuclear Regulatory Agency
OCRWM	Office of Civilian Radioactive Waste Management
TSPA	Total System Performance Assessment

ATTACHMENT II

SPREADSHEET CALCULATION TO OPTIMIZE THE GOODNESS OF FIT OF THE SINGLE EXPONENTIAL REPRESENTATION OF BDCF ABSTRACTIONS DUE TO RADIONUCLIDE BUILD-UP IN SOIL AS A RESULT OF PERIODS OF PREVIOUS IRRIGATION WITH CONTAMINATED GROUNDWATER

Exponential Fitting Template V1_0

File name EXPONENTIAL FITTING ROUTINE V1_0.XLS Version 1.0

OVERVIEW

This attachment provides documentation for the Excel Spreadsheet template routine used in this AMR to determine the parameters that are associated with the optimal fit for the exponential representation of the time evolution of the abstracted distribution mean of the BDCFs over periods of previous irrigation. The abstracted data were obtained from DTN MO0003SPASEA08.005.

The Excel Spreadsheet template routine that was used for all of the data in the AMR and DTN was worksheet named *Exponential Fitting Routine V1_0 Version 1.0* with file name *EXPONENTIAL FITTING ROUTINE V1_0.xls.*

This template routine was developed using Microsoft Excel 97 SR-2 running on a DELL POWEREDGE 2200 (Control Number 112375) with the Microsoft Windows NT operating system.

DESCRIPTION OF THE TEMPLATE

The Excel routine developed to process the multiple files of source data was classed as a template. The use of the word template was justified as a single Excel file (with extension .xls) was developed that contained the function and the "instructions" could be "cut and pasted" into multiple worksheets containing the data. The resulting worksheets were given names that uniquely identified the radionuclide for which the data is processed in each sheet.

The template is structured into three compartments. These compartments are discussed sequentially as processed by Excel. The following tables show the equations entered in the cells of the template.

Table II- 1 shows the input portion of the template. Table II-1 shows data that are those applicable to ^{90}Sr. It should be noted that this and some following tables are copied from Excel with the display in "show equation mode". In this mode the full value of each number is displayed as shown in the spreadsheet memory. The user cannot define the number of significant places to be shown. This example was selected here as only ^{90}Sr was abstracted as a shifted lognormal distribution. All the other abstraction were lognormal and as a result did have a "shift" i.e., for the other radionuclides column B is blank (effectively full of zeros). Cell C:2 contained the identifier for the radionuclide under consideration. The six sets (one for each period of previous period of irrigation) of parameters to describe the abstracted statistical distributions for the radionuclide identified in C:2 are to be copied into cells B6:F11. The input is distributed by column as follows.

- Column A was intentionally left blank.
- Column B contains the shift (as noted above this only applicable to the shifted lognormal distribution).
- Column C contains the serial number of period of previous irrigation (this is for reference and is not used in calculations).

- Column D contains the number of years of previous irrigation appropriate that the radionuclide under consideration for the period identified in column C.
- Column E contain the mean value of the (lognormal or shifted lognormal) distribution.
- Column F contain the standard deviation of the (lognormal or shifted lognormal) distribution.

Table II- 1 The Parameter Input Section of the Template.

	B	C	D	E	F
2		Sr90			
3			Scaling Factor	0.0001	
4					
5	Shift	Period #	Years Irrigation	Mean	SD
6	1.18463005629477	1	0	-0.604541501404625	0.594369296831068
7	1.2529144109665	2	5	-0.254711781720193	0.704607442049037
8	1.34703351323365	3	12	-0.0767672713229234	0.82270272781682
9	1.41004387838877	4	21	0.0339240920336918	0.912178606572511
10	1.49539999666267	5	33	0.0639163252711115	0.983475524342991
11	1.52479520935758	6	53	0.114288654664884	1.00647093134591

The second portion of the template is shown in Table II- 2. This is where the expression derived in Eq. 8 in Section 6.1 is fitted to the abstracted data. As the equations derived in section 6.1, apply to the actual values of the BDCF parameter and not to the logarithm of that parameter, the first calculation in column H is to represent the abstracted parameters as an actual BDCF. This is achieved by raising e, the base of the natural logarithm, to the power of the parameter and in the case of a shifted lognormal distribution adding in the shift.

Column J and L contain the instructions that allow the user to calculate the values of the parameters in Eq. 6 that provide the optimum fit to the time evolution of the mean of the BDCF abstractions.

- Cells J1:J3 are loaded with estimates of the three parameters defined in Eq. 6, i.e., B, C, and D respectively.
- Cells J6:J11 contain the expression (Eq. 6) required to generate the predicted value of the BDCF value derived in the corresponding row of column H.
- Cells L6:L11 contain the square of the differences between the actual value and value predicted by Eq. 6.
- Cell L:13 contain the sum of the values in cells L6:L11, i.e., the sum of the squares of the differences between the actual and predicted values.

By varying the parameters in cells J1:J3 such that cell L13 attains a minimum will provide the best estimate of the parameters in Eq. 6 according to the least squares fitting criterion. This optimization process is discussed in the next Section (Use of the Template).

The final part of the template is shown in Table II- 3. This section evaluates, in column N, the maximum relative deviation between actual and the optimized predicted values. Table II- 3 is self-explanatory and required no discussion.

Table II- 2 Exponential Fitting Portion of the Template.

	H	I	J	K	L
1		B	13.860083494729		
2		C	1.73815001635026		
3		D	0.0661919189368523		=+J3*J1
4					
5	exp(Mean)+Off-set		Predicted		Difference^2
6	=+EXP(E6)+B6		=+$J$2+$J$3*(1-EXP(-D6/$J$1))*$J$1		=+(H6-J6)^2
7	=+EXP(E7)+B7		=+$J$2+$J$3*(1-EXP(-D7/$J$1))*$J$1		=+(H7-J7)^2
8	=+EXP(E8)+B8		=+$J$2+$J$3*(1-EXP(-D8/$J$1))*$J$1		=+(H8-J8)^2
9	=+EXP(E9)+B9		=+$J$2+$J$3*(1-EXP(-D9/$J$1))*$J$1		=+(H9-J9)^2
10	=+EXP(E10)+B10		=+$J$2+$J$3*(1-EXP(-D10/$J$1))*$J$1		=+(H10-J10)^2
11	=+EXP(E11)+B11		=+$J$2+$J$3*(1-EXP(-D11/$J$1))*$J$1		=+(H11-J11)^2
12					
13				SS	=SUM(L6:L11)

Table II- 3 Portion of the Template that Calculates the Maximum Relative Deviation Between Actual and the Optimized Eq. 6 Fit.

	J	K	L	M	N
1	13.860083494729				
2	1.73815001635026				
3	0.0661919189368523		=+J3*J1		
4					
5	Predicted		Difference^2		
6	=+$J$2+$J$3*(1-EXP(-D6/$J$1))*$J$1		=+(H6-J6)^2		=+(H6-J6)/J6
7	=+$J$2+$J$3*(1-EXP(-D7/$J$1))*$J$1		=+(H7-J7)^2		=+(H7-J7)/J7
8	=+$J$2+$J$3*(1-EXP(-D8/$J$1))*$J$1		=+(H8-J8)^2		=+(H8-J8)/J8
9	=+$J$2+$J$3*(1-EXP(-D9/$J$1))*$J$1		=+(H9-J9)^2		=+(H9-J9)/J9
10	=+$J$2+$J$3*(1-EXP(-D10/$J$1))*$J$1		=+(H10-J10)^2		=+(H10-J10)/J10
11	=+$J$2+$J$3*(1-EXP(-D11/$J$1))*$J$1		=+(H11-J11)^2		=+(H11-J11)/J11
12					
13		SS	=SUM(L6:L11)		=+MAX(N6:N11)
14					=-MIN(N6:N11)
15					=+MAX(N13:N14)

Data – Template Integration

The abstracted BDCF distribution file was opened. Additional worksheets (one for each radionuclide) were added. Template file was opened, the used cells (A1:N15) were highlighted and COPIED on to the clip-board. The clipboard was then pasted into cell A:1 of each of the new worksheets. The TAB of each of the additional worksheets were given a unique name (the radionuclide to be considered in that worksheet). The appropriate data was copied from the summary sheet containing all the abstracted data into the input cells of the template.

Initial Action

The initial estimates of the parameters *B*, *C*, and *D* were loaded into cells J1:J3. It should be noted that these estimates need only be approximate. Reasonable estimates could be obtained as follows

- For C (cell J:2), the value of BDCF for irrigation period 1.
- For B (cell J:1), a value of the time corresponding to about midway between minimum and maximum BCDFs.
- For D (cell J:3), a value that is approximately given by the BDCF for the period 6 less C all divided by B.

Optimization

The Excel "Solver" was initiated. This is found on the pull down menu for "Tools"
In the "Solver Parameters" box, the following actions are taken.

1. "Set Target Cell" to L13.
2. Set the "Equal to" radio button to "Min".
3. Set the "By Changing Cells" to J1:J3.
4. Push the "Options" button and check the "Use Automatic Scaling" box, push "OK" button.
5. Push the "Solve" button.

If the "Solver" finds a minimum, accept the values.
If the "Solver" is unable to converge to a solution, reset the values to their initial values.
Repeat the sequence 1 to 5 above but in item 3, select only one of the parameters to vary. Repeat the last step but using a different parameter to vary. Once solutions have been reached by varying each parameter in turn, vary two at a time. Finally use the initial approach and generate a solution by varying all three parameters together.

Demonstration of functionality

To provide a demonstration that the template performs the required fitting of Eq. 6 to the data, a simple test was conducted. The test used six data points derived from Eq. 6 by using a Excel with predefined parameters (B, C, and D). The initial conditions are shown in Table II- 4, as are the exact values for the (artificial) BDCFs.

Table II- 4 Starting Conditions for Template Test

	C	D	E	F	G	H	I	J	K	L
1		B	100				B	50		
2	TEST	C	1				C	0.8		
3		D	1.E-02				D	0.01		5.00E-01
4										
5	Period #	Years Irrigation	Mean	SD		Test Values		Predicted		Difference^2
6	1	0				1		0.8		4.00E-02
7	2	25				1.22119922		0.99673467		5.04E-02
8	3	50				1.39346934		1.116060279		7.70E-02
9	4	100				1.63212056		1.232332358		1.60E-01
10	5	200				1.86466472		1.290842181		3.29E-01
11	6	400				1.98168436		1.299832269		4.65E-01
12										
13									SS	1.12E+00

Following the use of the built-in SOLVER function as directed above provides the values shown in Table II- 5. To within the desired accuracy the template determined a good approximation to the expected results. By using the Excel format capability to only show two decimal place would have indicated an exact fit to the know solution.

Table II- 5 Optimized Conditions after use of SOLVER on Template Test

	C	D	E	F	G	H	I	J	K	L
1		B	100				B	99.99668358		
2	TEST	C	1				C	0.999985481		
3		D	1.E-02				D	0.010000381		1.00E+00
4										
5	Period #	Years Irrigation	Mean	SD		Test Values		Predicted		Difference^2
6	1	0				1		0.999985481		2.11E-10
7	2	25				1.22119922		1.221192245		4.86E-11
8	3	50				1.39346934		1.393466818		6.36E-12
9	4	100				1.63212056		1.632121356		6.35E-13
10	5	200				1.86466472		1.864663435		1.64E-12
11	6	400				1.98168436		1.981677109		5.26E-11
12										
13									SS	3.21E-10

Conclusion

As further evidence that the integrated routine functions as expected is provided by Table II- 3, in Section 6.4. Here it was shown that the template when used with the actual BDCF data gave over all five radionuclide data sets a maximum relative deviation of less than one percent. The agreement, bearing in mind the stochastic source of the BDCFs, demonstrated the functionality of the methodology employed.