CRWMS/M&O

Calculation Cover Sheet

Complete only applicable items.

1. QA: L

Page: 1 Of: 6

2. Calculation Title Fitting of the Data for Diffusion Coefficients in Unsaturated Porous Media			
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Title: Fitting of the Data for Diffusion Coefficients in Unsaturated Porous Media

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Title: **Fitting of the Data for Diffusion Coefficients in Unsaturated Porous Media**

Document Identifier: B000000000-01717-0210-00026 REV 00

Originator: **Bryan E. Bullard**

Checker: **Bryan Dunlap**

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Draft Date: **August 6, 1998**

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1.0 Purpose

The purpose of this calculation is to evaluate diffusion coefficients in unsaturated porous media for use in the TSPA-VA analyses. Using experimental data, regression techniques were used to curve fit the diffusion coefficient in unsaturated porous media as a function of volumetric water content. This calculation substantiates the model fit used in Total System Performance Assessment-1995 An Evaluation of the Potential Yucca Mountain Repository (TSPA-1995), Section 6.5.4.

2.0 Method

Using an unsaturated flow apparatus based on open-flow centrifugation, Conca and co-workers at Pacific Northwest National Laboratories measured aqueous diffusion coefficients in a wide spectrum of geologic materials at varying degrees of water saturation. It was suggested from their study that diffusion coefficients are functions primarily of water content and not materials characteristics. The data set and model used were as given in TSPA-1995, Section 6.5.4. The model was fit by a least squares method. The functional form is expressed as

$$\log D_p = a + b \log \phi + \varepsilon$$

Where D_p is the diffusion coefficient (cm²/sec) and ϕ is the volumetric water content in percent and ε is random error. The model parameters a and b are determined from the least squares fit. The data set (DTN: MO9807SPA00026.000) was supplied from Engel (1995). The data is not qualified and results derived from it should be considered "to be verified" under TBV-377. A general discussion related to the data set can be found in Conca and Wright (1992).

3.0 Assumptions

The following assumptions were made:

1. The model predictions assume that the log base 10 transformed output variables have identical error distributions and that these error distributions are normally distributed. The basis of this assumption is supported by the data gathering method and analysis of the residuals. This assumption is used throughout the calculation.
2. The model as given in TSPA-1995 is assumed to be of the proper functional form. This assumption is used throughout the calculation.

4.0 Use of Computer Software

4.1. Software Approved for QA Work

N/A.

4.2. Software Routines

The software used was Mathcad 7 Professional. The type of computer used was a Dell PowerEdge 2200 with a Pentium II - 266 MHz CPU, 128 MB of RAM, in a Windows NT 4.0 operating system.

Mathcad 7 is an appropriate application because it provides a wide variety of mathematical functions that are necessary for the calculations used. Also, the program provides ease of display of equations and rationale employed, which eliminates the need to attach extra explanation and justification for the specific methodology.

5.0 Calculation

All calculations use data (DTN: MO9807SPA00026.000) contained in Engel (1995). This input data is "to be verified" (TBV-377) and thus, the results of this calculation should be considered "to be verified."

5.1. Description

The calculation inputs consist of 177 observations of diffusion coefficients for various degrees of water saturation, the source of the data is shown in Attachment II, Engel (1995), (values are also shown in Attachment I, Section B – Data Listing on pages I-4 to I-10).

See Attachment I, Section A for a further description of the calculation.

5.2. Procedure

See Attachment I, Section A.

6.0 Results

All results are to be considered "to be verified" (TBV-377) as this calculations uses as inputs data (DTN: MO9807SPA00026.000) contained in Engel (1995). A predicted value of an individual observation will be given by the following equation and standard deviation below

$$\log D_p = a + b \log \phi + z \cdot \text{std}(\phi)$$

$$\text{std}(\phi) = \sqrt{\Sigma_{00} + 2 \cdot \Sigma_{01} \cdot \log(\phi) + \Sigma_{11} \cdot \log(\phi)^2 + \sigma_e^2}$$

Where z is a standard normal, D_p is the diffusion coefficient (cm²/sec) and ϕ is the volumetric water content in percent. Numerical values for the model parameters from the regression fit are:

$$a = -8.254664, b = 1.89762, \sigma_e^2 = 0.086845, \Sigma = \begin{bmatrix} 2.468868\text{E}-3 & -2.052563\text{E}-3 \\ -2.052563\text{E}-3 & 2.129701\text{E}-3 \end{bmatrix}$$

For further details see Attachment I, Section A.

Title: Fitting of the Data for Diffusion Coefficients in Unsaturated Porous Media**Document Identifier:** B00000000-01717-0210-00026 REV 00 (*August 6, 1998*)**Page 6 of 6**

7.0 References

Conca, J. L., and J. Wright, 1992. "Diffusion and Flow in Gravel Soil, and Whole Rock," Applied Hydrogeology, Vol. 1, pp. 5-24. TIC#: 224081.

Engel, D., 1995 Memo to J.H. Lee, January 30. DTN: MO90807SPA00026.000. TBV-377.

M&O (Civilian Radioactive Waste Management System, Management and Operating Contractor [CRWMS M&O]), 1995. Total System Performance Assessment-1995: An Evaluation of the Potential Yucca Mountain Repository, B00000000-01717-2200-00136, Rev. 01, Las Vegas, NV. MOL.19960724.0188.

8.0 Attachments

ATTACHMENT	TITLE	NUMBER OF PAGES
I	Diffusion Coefficient in Unsaturated Porous Media	11
II	Memo to J.H. Lee, January 30	5

Attachment I - Diffusion Coefficient in Unsaturated Porous Media

Section A - Regression Calculation

Measured diffusion coefficients in a geologic materials at varying degrees of water saturation show a functional relationship between the diffusion coefficient in unsaturated porous media and the volumetric water content.

The following data DTN: MO9807SPA00026.000 (input file data3) originates from an e-mail, Attachment II (Engel, 1995). The data matrix is displayed in Section B - Data Listing on pages I-5 to I-11. Four points have been removed consisting of the data set labeled benton/sand, density=2.00. The data is not qualified and all results are "to be verified" under TBV-377.

data := D:\diffus\data3 bentonsand :=
$$\begin{bmatrix} 1.3 \cdot 10^1 & 5 \cdot 10^{-8} \\ 1.3 \cdot 10^1 & 4 \cdot 10^{-8} \\ 1.3 \cdot 10^1 & 1.6 \cdot 10^{-8} \\ 1.3 \cdot 10^1 & 3 \cdot 10^{-9} \end{bmatrix}$$
 • Points removed from regression analysis, see graph below.

rows(data) = 177 cols(data) = 2 • 177 data pairs were used in the regression fit.

i := 0..rows(data) - 1 • row index for values in data matrix, indexing starts with zero.

$y_i := \log(\text{data}_{i,1})$ • y values are $\log_{10}(D_p)$, where D_p is pore diffusion in cm^2/s

$x_i := \log(\text{data}_{i,0})$ • x values are $\log_{10}(\phi)$, where ϕ is percent volumetric water content

Create system of equations of form $y = a + bx$ to solve in matrix form

$$X_{1,0} := 1 \quad X_{1,1} := x_i$$

$$\text{invXX} := (X^T \cdot X)^{-1}$$

verification using built in functions

$$B := \text{invXX} \cdot X^T \cdot y \quad B = \begin{bmatrix} -8.254664 \\ 1.89762 \end{bmatrix}$$

$$\text{intercept}(x, y) = -8.254664$$

$$\text{slope}(x, y) = 1.89762$$

$$a := B_{0,0} \quad b := B_{1,0}$$

$$\sigma^2 := \frac{(y^T \cdot y - B^T \cdot X^T \cdot y)}{(\text{rows}(X) - 1)}$$

• Estimate of the residual variance. Note that for an unbiased estimator the denominator term should be minus two not one, the "erroneous" value is maintained for consistency with the values used in TSPA-VA. This change alters the result in the error variance at the fourth decimal place and the fifth decimal place for the variance-covariance matrix. (Corrected values are calculated on page I-4, correction to be made in REV. 01 of this calculation.)

$$\sigma^2 = 0.086845$$

$$\Sigma := \sigma^2 \cdot \text{invXX}$$

$$\Sigma = \begin{bmatrix} 2.468868 \cdot 10^{-3} & -2.052563 \cdot 10^{-3} \\ -2.052563 \cdot 10^{-3} & 2.129701 \cdot 10^{-3} \end{bmatrix}$$

• Estimate of the variance-covariance matrix for coefficient vector B.

$$\text{Syo}(x) := \sqrt{\Sigma_{0,0} + 2 \cdot \Sigma_{0,1} \cdot x + \Sigma_{1,1} \cdot x^2 + \sigma^2_{0,0}} \quad \text{• Standard deviation for an individual predicted value of } y \text{ given at } x.$$

$$y_o(x, z) := a + b \cdot x + z \cdot \text{Syo}(x)$$

$$n := 60 \quad \text{high} := \max(x) \quad \text{low} := \min(x) \quad \text{ii} := 0..n-1 \quad \text{xx}_{\text{ii}} := \text{low} + \left(\frac{\text{high} - \text{low}}{n-1} \right) \cdot \text{ii}$$

- Note one point (1.6e-1, 4.31e-9) appears as an outlier at the lower limit of percent volumetric water content. Solid line is mean value and dashed lines are ± 2 std.

$\text{pow10}(y) := 10^y$ • Create a function to raise argument to power base 10.

Compare below with Figure 6.5-6 in TSPA-1995, page 6-55

- Model Estimation and the Uncertainty for the Diffusion Coefficient in Porous Geologic Media as a Function of the Volumetric Water Content. The raw data for a suite of geological materials were kindly provided by Jim Conca through David Engel at PNL (Engel, 1995).

Summary

$$a = -8.254664 \quad b = 1.89762 \quad \sigma\epsilon^2 = 0.086845 \quad \Sigma = \begin{bmatrix} 2.468868 \cdot 10^{-3} & -2.052563 \cdot 10^{-3} \\ -2.052563 \cdot 10^{-3} & 2.129701 \cdot 10^{-3} \end{bmatrix}$$

Pore diffusivity and effective diffusion coefficient (D_{eff}) in m^2/s given ϕ and a standard normal value, z . Note: y values are $\log_{10}(D_p)$, where D_p is pore diffusion in cm^2/s . x values are $\log_{10}(\phi)$, where ϕ is percent volumetric water content.

$$\text{Sy}\sigma(x) := \sqrt{\Sigma_{0,0} + 2 \cdot \Sigma_{0,1} \cdot x + \Sigma_{1,1} \cdot x^2 + \sigma\epsilon^2_{0,0}}$$

$$\text{yo}(x, z) := a + b \cdot x + z \cdot \text{Sy}\sigma(x)$$

$$D_{\text{pore}}(\phi, z) := \text{pow10}(\text{yo}(\log(\phi), z)) \cdot 10^{-4}$$

$$D_{\text{eff}}(\phi, z) := \frac{\phi \cdot D_{\text{pore}}(\phi, z)}{100}$$

Corrected values in the calculation of the residual variance

The a and b coefficient values remain unchanged.

$$\sigma\epsilon^2 := \frac{(y^T \cdot y - B^T \cdot X^T \cdot y)}{(\text{rows}(X) - 2)}$$

$$\sigma\epsilon^2 = 0.087341$$

$$\Sigma := \sigma\epsilon^2_{0,0} \cdot \text{inv}XX$$

$$\Sigma = \begin{bmatrix} 2.482976 \cdot 10^{-3} & -2.064292 \cdot 10^{-3} \\ -2.064292 \cdot 10^{-3} & 2.14187 \cdot 10^{-3} \end{bmatrix}$$

• Estimate of the residual variance. The denominator term is number of cases minus two, demonstrating that the changes discussed previously (I-2) alter the result in the error variance at the fourth decimal place and the fifth decimal place for the variance-covariance matrix. Correction to be made in Rev. 01 of this calculation.

• Estimate of the variance-covariance matrix for coefficient vector B.

$$S_{yO}(x) := \sqrt{\Sigma_{0,0} + 2 \cdot \Sigma_{0,1} \cdot x + \Sigma_{1,1} \cdot x^2 + \sigma\epsilon^2_{0,0}}$$

• Standard deviation for an individual predicted value of y given at x.

$$yO(x, z) := a + b \cdot x + z \cdot S_{yO}(x)$$

• Note one point (1.6e-1, 4.31e-9) appears as an outlier at the lower limit of percent volumetric water content. Solid line is mean value and dashed lines are ± 2 std.

Section B - Data Listing (DTN: MO9807SPA00026.000)

Volumetric Water Pore Diffusion
Content (%) D (cm²/s)

Data is "to be verified" and all results based on this
dat set should be tracked with TBV-377.

data =

12.700000	4.900000•10 ⁻⁷
11.100000	3.720000•10 ⁻⁷
10.500000	3.300000•10 ⁻⁷
8.800000	2.300000•10 ⁻⁷
8.000000	1.980000•10 ⁻⁷
7.300000	1.600000•10 ⁻⁷
28.200000	3.500000•10 ⁻⁶
32.300000	4.600000•10 ⁻⁶
11.760000	4.800000•10 ⁻⁷
8.320000	4.100000•10 ⁻⁷
23.100000	2.400000•10 ⁻⁶
16.700000	6.600000•10 ⁻⁷
13.900000	7.800000•10 ⁻⁷
11.600000	5.400000•10 ⁻⁷
8.600000	3.200000•10 ⁻⁷
7.600000	2.600000•10 ⁻⁷
7.400000	2.500000•10 ⁻⁷
25.400000	2.500000•10 ⁻⁶
23.100000	1.900000•10 ⁻⁶
18.900000	1.200000•10 ⁻⁶
17.500000	1.100000•10 ⁻⁶
17.000000	1.200000•10 ⁻⁶
24.000000	2.900000•10 ⁻⁶
21.000000	2.340000•10 ⁻⁶
18.300000	1.900000•10 ⁻⁶
17.300000	1.760000•10 ⁻⁶

-<

• Start of Data Set 1

16.000000	$1.470000 \cdot 10^{-6}$
18.800000	$1.600000 \cdot 10^{-6}$
17.100000	$8.200000 \cdot 10^{-7}$
12.000000	$2.400000 \cdot 10^{-7}$
14.700000	$9.000000 \cdot 10^{-7}$
14.400000	$5.200000 \cdot 10^{-7}$
8.100000	$1.700000 \cdot 10^{-7}$
5.900000	$9.300000 \cdot 10^{-8}$
4.900000	$7.200000 \cdot 10^{-8}$
7.700000	$1.100000 \cdot 10^{-7}$
5.830000	$1.230000 \cdot 10^{-7}$
5.400000	$7.600000 \cdot 10^{-8}$
3.570000	$3.370000 \cdot 10^{-8}$
6.900000	$6.000000 \cdot 10^{-8}$
3.340000	$2.600000 \cdot 10^{-8}$
3.700000	$3.700000 \cdot 10^{-8}$
5.300000	$2.400000 \cdot 10^{-8}$
14.400000	$4.500000 \cdot 10^{-7}$
12.500000	$2.900000 \cdot 10^{-7}$
12.300000	$4.400000 \cdot 10^{-7}$
11.700000	$2.600000 \cdot 10^{-7}$
12.300000	$3.600000 \cdot 10^{-7}$
10.300000	$2.100000 \cdot 10^{-7}$
11.200000	$5.480000 \cdot 10^{-7}$
7.600000	$1.100000 \cdot 10^{-7}$
3.330000	$6.350000 \cdot 10^{-8}$
3.140000	$3.060000 \cdot 10^{-8}$
2.290000	$1.090000 \cdot 10^{-8}$
1.420000	$1.950000 \cdot 10^{-9}$

7.600000	$2.690000 \cdot 10^{-7}$
6.930000	$1.500000 \cdot 10^{-7}$
5.510000	$7.680000 \cdot 10^{-8}$
3.270000	$2.790000 \cdot 10^{-8}$
3.200000	$1.350000 \cdot 10^{-8}$
40.000000	$6.900000 \cdot 10^{-6}$
3.700000	$6.600000 \cdot 10^{-8}$
2.200000	$3.630000 \cdot 10^{-8}$
1.000000	$1.090000 \cdot 10^{-8}$
0.810000	$3.800000 \cdot 10^{-9}$
5.100000	$1.320000 \cdot 10^{-7}$
1.500000	$1.390000 \cdot 10^{-8}$
1.000000	$7.300000 \cdot 10^{-9}$
0.730000	$4.400000 \cdot 10^{-9}$
4.200000	$5.940000 \cdot 10^{-8}$
1.700000	$6.600000 \cdot 10^{-9}$
1.300000	$3.300000 \cdot 10^{-9}$
4.000000	$5.220000 \cdot 10^{-8}$
49.000000	$6.090000 \cdot 10^{-6}$
0.500000	$1.650000 \cdot 10^{-9}$
0.520000	$2.600000 \cdot 10^{-9}$
0.530000	$3.480000 \cdot 10^{-9}$
0.550000	$4.420000 \cdot 10^{-9}$
0.790000	$6.660000 \cdot 10^{-9}$
0.930000	$1.180000 \cdot 10^{-8}$
1.400000	$1.590000 \cdot 10^{-8}$
2.170000	$2.770000 \cdot 10^{-8}$
6.000000	$8.920000 \cdot 10^{-8}$

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4.600000	$6.210000 \cdot 10^0$
3.100000	$3.300000 \cdot 10^{-8}$
2.500000	$2.500000 \cdot 10^{-8}$
1.900000	$8.600000 \cdot 10^{-9}$
6.300000	$1.060000 \cdot 10^{-7}$
38.540000	$4.334000 \cdot 10^{-6}$
10.050000	$3.510000 \cdot 10^{-7}$
10.210000	$3.540000 \cdot 10^{-7}$
11.130000	$4.270000 \cdot 10^{-7}$
12.720000	$5.320000 \cdot 10^{-7}$
14.580000	$6.820000 \cdot 10^{-7}$
21.590000	$1.288000 \cdot 10^{-6}$
10.260000	$3.340000 \cdot 10^{-7}$
11.190000	$4.190000 \cdot 10^{-7}$
12.020000	$4.470000 \cdot 10^{-7}$
12.320000	$4.500000 \cdot 10^{-7}$
13.070000	$4.770000 \cdot 10^{-7}$
13.880000	$5.390000 \cdot 10^{-7}$
14.170000	$5.520000 \cdot 10^{-7}$
16.140000	$6.820000 \cdot 10^{-7}$
9.240000	$2.550000 \cdot 10^{-7}$
9.640000	$3.070000 \cdot 10^{-7}$
10.350000	$3.400000 \cdot 10^{-7}$
11.370000	$4.270000 \cdot 10^{-7}$
9.240000	$2.550000 \cdot 10^{-7}$
9.560000	$3.000000 \cdot 10^{-7}$
10.240000	$3.300000 \cdot 10^{-7}$
12.160000	$4.090000 \cdot 10^{-7}$
14.100000	$5.120000 \cdot 10^{-7}$

18.920000	$8.190000 \cdot 10^{-7}$
10.910000	$3.620000 \cdot 10^{-7}$
11.400000	$4.120000 \cdot 10^{-7}$
12.690000	$4.370000 \cdot 10^{-7}$
14.360000	$4.500000 \cdot 10^{-7}$
16.520000	$5.450000 \cdot 10^{-7}$
21.530000	$1.232000 \cdot 10^{-6}$
9.750000	$3.200000 \cdot 10^{-7}$
10.110000	$3.620000 \cdot 10^{-7}$
11.100000	$4.220000 \cdot 10^{-7}$
12.270000	$5.050000 \cdot 10^{-7}$
14.820000	$6.540000 \cdot 10^{-7}$
19.370000	$9.890000 \cdot 10^{-7}$
8.350000	$2.150000 \cdot 10^{-7}$
20.800000	$3.580000 \cdot 10^{-6}$
33.800000	$1.344000 \cdot 10^{-5}$
35.800000	$1.568000 \cdot 10^{-5}$
25.300000	$5.824000 \cdot 10^{-6}$
31.700000	$1.232000 \cdot 10^{-5}$
20.390000	$4.194400 \cdot 10^{-6}$
25.700000	$9.259040 \cdot 10^{-6}$
43.440000	$1.020320 \cdot 10^{-5}$
39.320000	$1.360800 \cdot 10^{-5}$
39.530000	$1.131200 \cdot 10^{-5}$
66.300000	$1.830000 \cdot 10^{-5}$
30.900000	$1.510000 \cdot 10^{-6}$
28.500000	$1.000000 \cdot 10^{-6}$
42.500000	$3.220000 \cdot 10^{-6}$

13.000000	$7.940000 \cdot 10^{-1}$
41.960000	$5.800000 \cdot 10^{-6}$
0.949000	$2.500000 \cdot 10^{-8}$
0.160000	$4.310000 \cdot 10^{-9}$
0.819000	$8.300000 \cdot 10^{-9}$
17.320000	$2.755200 \cdot 10^{-6}$
33.800000	$1.344000 \cdot 10^{-5}$
35.800000	$1.568000 \cdot 10^{-5}$
25.300000	$5.824000 \cdot 10^{-6}$
31.700000	$1.232000 \cdot 10^{-5}$
15.920000	$2.083200 \cdot 10^{-6}$
17.270000	$2.564800 \cdot 10^{-6}$
18.190000	$3.363360 \cdot 10^{-6}$
18.540000	$3.438400 \cdot 10^{-6}$
19.600000	$4.194400 \cdot 10^{-6}$
20.390000	$4.194400 \cdot 10^{-6}$
14.240000	$1.383200 \cdot 10^{-6}$
11.650000	$5.895700 \cdot 10^{-7}$
14.540000	$2.027200 \cdot 10^{-6}$
17.110000	$3.595200 \cdot 10^{-6}$
18.850000	$4.681600 \cdot 10^{-6}$
12.050000	$9.221000 \cdot 10^{-7}$
14.180000	$2.191840 \cdot 10^{-6}$
11.960000	$8.880500 \cdot 10^{-7}$
13.000000	$1.036800 \cdot 10^{-6}$
14.060000	$1.828960 \cdot 10^{-6}$
25.700000	$9.259040 \cdot 10^{-6}$
43.440000	$1.020320 \cdot 10^{-5}$
39.320000	$1.360800 \cdot 10^{-5}$

• Where benton/sand was removed

• Data pair labeled Japanese cores mudstone (1.6e-1 4.31e-9). Outlier very close to 0.1% limit, suspect value.

• Start of Data Set 2.
Starting with pair (17.32, .027552e-4)

39.530000	$1.131200 \cdot 10^{-5}$
0.870000	$5.290000 \cdot 10^{-9}$
0.945000	$1.510000 \cdot 10^{-8}$
14.900000	$2.120000 \cdot 10^{-6}$
13.440000	$1.510880 \cdot 10^{-6}$
11.910000	$1.001390 \cdot 10^{-6}$
11.730000	$1.210000 \cdot 10^{-6}$
10.480000	$9.447000 \cdot 10^{-7}$

Memo to J.H. Lee, January 30
Engel, D., 1995

- Electronic memo from Engel to Lee January 30, 1995.
- Data Set 2 is in different units than Data Set 1. Units were inferred from TSPA-1995 analysis.
- Data has been assigned data tracking number (DTN: MO9807SPA00026.000).
- Not qualified data, results based on this data are "to be verified" under (TBV-377).

- Text of email follows:

To: Joon Lee
cc:
Subject: Re: Jim's D(eff) Raw Data

Joon,

Below are the data sets from Jim Conca. I did not have all of the information that you requested per data point, but this is what we got from Jim.

The first set contains volumetric water content and diff coeff. for different samples. The second set contain volumetric water content, diff coeff., and density for compacted bentonite. I will fax you a description of that data.

If you have any questions, please call,

Dave Engel

xx
Data Set 1
xx

Attached is the diffusion coefficient versus water content data (Figure 2) from Diffusion and Flow in Gravel, Soil, and Whole Rock by Jim Conca and Judith Wright (Applied Hydrology 1/92)

*

SAMPLE	Volumetric Water Content (%)	D (cm ² /s)
G-1 soil	1.27e+1	4.9e-7
4/12/89	1.11e+1	3.72e-7
K-saturated	1.05e+1	3.3e-7
8.8e+0	2.3e-7	
8e+0	1.98e-7	
7.3e+0	1.6e-7	
2.82e+1	3.5e-6	
3.23e+1	4.6e-6	

G-1 soil	1.176e+1	4.8e-7
3/13/89	8.32e+0	4.1e-7
2.31e+1	2.4e-6	
1.67e+1	6.6e-7	

G-3 soil	1.39e+1	7.8e-7
3/22/89	1.16e+1	5.4e-7
not saturated	8.6e+0	3.2e-7
7.6e+0	2.6e-7	
7.4e+0	2.5e-7	

G-4 soil	2.54e+1	2.5e-6
3/31/89 2.31e+1	1.9e-6	
not saturated	1.89e+1	1.2e-6
1.75e+1	1.1e-6	
1.7e+1 1.2e-6		

G-4 soil	2.4e+1	2.9e-6
4/5/89 2.1e+1	2.34e-6	
K-saturated	1.83e+1	1.9e-6
1.73e+1	1.76e-6	
1.6e+1 1.47e-6		

Solid Waste

Landfill soils

gravel	1.88e+1	1.6e-6
lower c. sand	1.71e+1	8.2e-7
upper c. sand	1.2e+1	2.4e-7
gravel	1.47e+1	9e-7
lower c. sand	1.44e+1	5.2e-7
upper c. sand	8.1e+0	1.7e-7

gravel	5.9e+0	9.3e-8
lower c. sand	4.9e+0	7.2e-8
upper c. sand	7.7e+0	1.1e-7
lower c. sand	5.83e+0	1.23e-7
gravel	5.4e+0	7.6e-8
lower c. sand	3.57e+0	3.37e-8
upper c. sand	6.9e+0	6e-8
lower c. sand	3.34e+0	2.6e-8
gravel	3.7e+0	3.7e-8
upper c. sand	5.3e+0	2.4e-8

fine sand 2	1.44e+1	4.5e-7
fine sand 1	1.25e+1	2.9e-7

fine sand 2	1.23e+1	4.4e-7
fine sand 1	1.17e+1	2.6e-7
fine sand 2	1.23e+1	3.6e-7
fine sand 1	1.03e+1	2.1e-7
fine sand 2	1.12e+1	5.48e-7
fine sand 1	7.6e+0	1.1e-7

tuff gravel

6.3-9.5mm	3.33e+0	6.35e-8
3.14e+0	3.06e-8	
2.29e+0	1.09e-8	
1.42e+0	1.95e-9	
7.6e+0 2.69e-7		

2-4 mm	6.93e+0	1.5e-7
5.51e+0	7.68e-8	
3.27e+0	2.79e-8	
3.2e+0 1.35e-8		
saturated	4e+1	6.9e-6

basalt gravel

4-6.3mm	3.7e+0	6.6e-8
2.2e+0	3.63e-8	
1e+0	1.09e-8	
8.1e-1	3.8e-9	
5.1e+0	1.32e-7	

6.3-9.5mm	1.5e+0	1.39e-8
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1e+0 7.3e-9
 7.3e-1 4.4e-9
 4.2e+0 5.94e-8

12.5-15mm 1.7e+0 6.6e-9
 1.3e+0 3.3e-9
 4e+0 5.22e-8

saturated 4.9e+1 6.09e-6

granite gravel
 6.3-9.5mm 5e-1 1.65e-9
 5.2e-1 2.6e-9
 5.3e-1 3.48e-9
 5.5e-1 4.42e-9
 7.9e-1 6.66e-9
 9.3e-1 1.18e-8
 1.4e+0 1.59e-8
 2.17e+0 2.77e-8

river gravel 6e+0 8.92e-8
 2.0-3.4mm 4.6e+0 6.21e-8
 3.1e+0 3.3e-8
 2.5e+0 2.5e-8
 1.9e+0 8.6e-9
 6.3e+0 1.06e-7

Trench 8
 soils
 density=1.59

saturated 3.854e+1 4.334e-6

unsaturated 1.005e+1 3.51e-7
 various run 1.021e+1 3.54e-7
 parameters 1.113e+1 4.27e-7

1.272e+1 5.32e-7
 1.458e+1 6.82e-7
 2.159e+1 1.288e-6

1.026e+1 3.34e-7
 1.119e+1 4.19e-7
 1.202e+1 4.47e-7
 1.232e+1 4.5e-7

1.307e+1 4.77e-7
 1.388e+1 5.39e-7
 1.417e+1 5.52e-7
 1.614e+1 6.82e-7

9.24e+0 2.55e-7
 9.64e+0 3.07e-7
 1.035e+1 3.4e-7
 1.137e+1 4.27e-7

9.24e+0 2.55e-7
 9.56e+0 3e-7
 1.024e+1 3.3e-7
 1.216e+1 4.09e-7
 1.41e+1 5.12e-7
 1.892e+1 8.19e-7

1.091e+1 3.62e-7

1.14e+1	4.12e-7
1.269e+1	4.37e-7
1.436e+1	4.5e-7
1.652e+1	5.45e-7
2.153e+1	1.232e-6

9.75e+0	3.2e-7
1.011e+1	3.62e-7
1.11e+1	4.22e-7
1.227e+1	5.05e-7
1.482e+1	6.54e-7
1.937e+1	9.89e-7

8.35e+0	2.15e-7
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Kunigel V1 Bentonite

various compaction	2.08e+1	3.58e-6
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3.38e+1	1.344e-5
3.58e+1	1.568e-5
2.53e+1	5.824e-6
3.17e+1	1.232e-5

2.039e+1	4.1944e-6
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2.57e+1	9.25904e-6
4.344e+1	1.02032e-5
3.932e+1	1.3608e-5
3.953e+1	1.1312e-5

unc. bentonite density = 1.21	6.63e+1	1.83e-5
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Calico Hills	3.09e+1	1.51e-6
whole rock	2.85e+1	1e-6

benton:basalt
25:75

density = 1.64	4.25e+1	3.22e-6
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bentonite Tc	1.3e+1	7.94e-7
density = 2.00		

benton/sand
density = 2.00

Cs	1.3e+1	5e-8
Np	1.3e+1	4e-8
U	1.3e+1	1.6e-8
Am	1.3e+1	3e-9

Japanese cores

tuff 1.34 g/cc	4.196e+1	5.8e-6
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basalt 2.90 g/cc	9.49e-1	2.5e-8
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mudstone 2.72 g/cc	1.6e-1	4.31e-9
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granite 2.60 g/cc	8.19e-1	8.3e-9
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0A: N

Affected Organization: M40 Prepared - 18-JUN-98:13:10:26	Yucca Mountain Site Characterization Project Planning and Control System (PACS) Procurement Preparation Sheet (PPS)	DE-ACO .RW00134 Page - 1 Dollars in Thousands (Esc.)
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PWBS Element: 1.2.5.4 Product: 1122 Control Account: 12541122	Performance Assessment TSPA Documentation TSPA Documentation	Start Date: 01-oct-1997 Finish Date: 18-mar-1999 QA - YES
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	Prior	FY1998	FY1999	FY2000	FY2001	FY2002	FY2003	FY2004	FY2005	FY2006	FY2007	Future	At Complete
Annual Budget	0	948	257	0	0	0	0	0	0	0	0	0	1205

Statement of Work

The following work shall be controlled in accordance with approved implementing procedures identified on the current, OCRWM-accepted Requirements Traceability Network Matrix.

The approach, assumptions, models and model abstractions, scenarios, parameters, results, sensitivity analyses, and conclusions and implications for additional site characterization and design for TSPA-VA will be documented in a series of technical report suitable for external review by various types of external groups. These reports will be a comprehensive summation of all the relevant inputs and outputs plus discussion of the degree of conservatism in the analyses. However, each document in the series will be produced for a different audience. The three different audiences are expected to be the regulator, the scientific community, and the public. Different degrees of detail and illustration will be developed as appropriate for each audience. Documentation may be included in the form of hardcopy or electronic files, suitable for distribution on the WWW. Some of the sections of this document shall be prepared in other activities (in particular the abstraction/testing activities, the scenario identification and screening activity, and the TSPA -VA software upgrade and documentation activity). The Work Packages are as follows:

Document Results for TSPA-VA
 TSPA Documentation Illustration and Communication
 Management Integration

TECHNICAL BASELINE DOCUMENTS

Work is to be performed in accordance with the latest revision of the following technical documents:

Level 1 - Program:
 Not Applicable

Level 2 - YMSCO:
 Mined Geologic Disposal System Requirements Document

Level 3 - WAST:
 Not Applicable

Work Package	Title
12541122M1	Document Results for TSPA-VA
12541122M2	TSPA-VA Doc Illustration & Communication

DELIVERABLES		
Deliv ID	Description/Completion Criteria	Due Date
SL230AM3	Complete TSPA-VA Analyses Technical Basis Doc Criteria - Description:	21-aug-1998

12541122 TSPA Documentation (continued)

DELIVERABLES

Deliv ID	Description/Completion Criteria	Due Date
CR98/023	<p>This Technical Basis document will support the TSPA-VA volume by providing documentation of the use of total system models drawn from process-level models (developed in the site-characterization, environmental and design programs) from subsystem models developed in other PA activities and from models developed from other data sources where required to adequately represent the total system to perform analyses of radionuclide release and ultimately the peak concentration, dose or risk associated with these releases to the biosphere. Results of the TSPA that feed EBS design, WP design, other design/engineering activities, and site characterization activities will be discussed in order to allow these programs to update process-level models (if necessary) for input into the TSPA analysis for LA. A stand alone report, fully documented as described in the TSPA Methodology and Assumptions document and suitable for external peer review will be produced. This document will follow similar outlines to previous TSPA iterations, but be more encompassing to evaluate the potential effects of alternative processes and process interactions on subsystem performance.</p> <p>Completion Criteria: This deliverable shall be prepared in accordance with OCRWM approved quality assurance procedures implementing requirements of the Quality Assurance Requirements Description. The product shall be developed on the basis of the best technical data, including both Q and non-Q data. The Q status of data used and cited in the report shall be appropriately noted or referenced. Within the report's Reference Section, references to data shall be used in the report shall include record Accession Numbers or Data Tracking Numbers when available.</p> <p>AcceptanceCriteria: Technical data contained within the deliverable and not already incorporated in the Geographic Nodal Information Study and Evaluation System (GENISES) shall be submitted for incorporation into the GENISES in accordance with YAP-SIII.3Q. Verification of technical data submittal compliance shall be demonstrated by including as part of the deliverable: 1) a copy of the Technical Data Information Form generated identifying the data in the Automated Technical Data Tracking system, and 2) a copy of the transmittal letter attached to the technical data transmittal to the GENISES Administrator. This deliverable shall be processed in accordance with YAP-7.1Q.</p>	

Approvals

S/R. ANDREWS
Preparer - print name

S/R. SPENCE
Technical Reviewer - print name

S/C. HAMPTON
QA Reviewer - print name

S/11/98
Preparer - signature Date

S/14/98
Technical Reviewer - signature Date

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QA Reviewer - signature Date