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10. Lead/Supervisor	Kurt R. Rautenstrauch	<i>Kurt Rautenstrauch</i>	9/8/99
11. Responsible Manager	Ronald A. Green	<i>Ronald A Green</i>	9/9/99

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CONTENTS

	Page
1. PURPOSE.....	5
2. QUALITY ASSURANCE.....	6
3. COMPUTER SOFTWARE AND MODEL USAGE.....	7
4. INPUTS.....	7
4.1 DATA.....	7
4.1.1 Mass Loading.....	7
4.1.2 Inhalation Exposure Time.....	9
4.1.3 Chronic Breathing Rate.....	9
4.1.4 Soil Exposure Time.....	9
4.1.5 Home Irrigation Rate.....	9
4.1.6 Duration of Home Irrigation.....	10
4.2 CRITERIA.....	10
4.3 CODES AND STANDARDS.....	10
5. ASSUMPTIONS.....	10
5.1 MASS LOADING.....	10
5.2 INHALATION EXPOSURE TIME.....	11
5.3 CHRONIC BREATHING RATE.....	12
5.4 SOIL EXPOSURE TIME.....	12
5.5 HOME IRRIGATION RATE.....	12
5.6 DURATION OF HOME IRRIGATION.....	13
6. ANALYSIS.....	13
6.1 MASS LOADING.....	13
6.2 INHALATION EXPOSURE TIME.....	14
6.3 CHRONIC BREATHING RATE.....	15
6.4 SOIL EXPOSURE TIME.....	16
6.5 HOME IRRIGATION RATE.....	17
6.6 DURATION OF HOME IRRIGATION.....	20
7. CONCLUSIONS.....	20
8. REFERENCES.....	22
8.1 DATA CITED.....	22
8.2 DOCUMENTS CITED.....	22
8.3 CODES, STANDARDS, AND REGULATIONS.....	25
8.4 PROCEDURES.....	25
APPENDIX A.....	27
APPENDIX B.....	31

FIGURES

	Page
1. Untransformed PM ₁₀ concentration data ($\mu\text{g}/\text{m}^3$) from Site 9, 10/3/92 to 12/30/97.	13
2. Log (base 10) transformed PM ₁₀ concentration data ($\mu\text{g}/\text{m}^3$) from Site 9, 10/3/92 to 12/30/97.	14

TABLES

1. Summary of inputs used in this analysis.	8
2. Time (hours/year) spent in contaminated and uncontaminated areas based on three lifestyle scenarios.	15
3. Average monthly temperature and solar radiation at YMP Site 9, monthly reference evapotranspiration (ET _r), and monthly crop coefficients and evapotranspiration for bermudagrass and tall fescue.	19
4. Summary of parameter values for GENII-S code input derived from analyses presented in this report.	21

1. PURPOSE

The purpose of this analysis and model report (AMR) is to select and justify values for six input parameters used by the computer code GENII-S (Leigh et al. 1993). The GENII-S code is being used to estimate radionuclide-specific biosphere dose conversion factors. The Civilian Radioactive Waste Management System Management and Operating Contractor (CRWMS M&O) Performance Assessment Organization will use the biosphere dose conversion factors to calculate potential radiation doses to a hypothetical human receptor group as part of the post-closure Total System Performance Assessment.

The six parameters evaluated in this analysis are for two of the three exposure pathways to humans considered to calculate biosphere dose conversion factors: inhalation and external exposure. The inhalation pathway evaluates inhalation of respirable, resuspended dust from contaminated soils. Three parameters for this pathway were analyzed in this report.

1. **Mass Loading (g/m^3)** — Mass loading is the mass of suspended particles per volume of air. This parameter is used to calculate the concentration of radionuclides in the air resulting from resuspension of soil contaminated by irrigation. Mass loading was estimated in this analysis directly from measurements of particulate matter ($\leq 10 \mu\text{m}$ in diameter) taken for the Yucca Mountain Site Characterization Project (YMP).
2. **Inhalation Exposure Time (hours/year)** — Inhalation exposure time is the amount of time a reference person inhales resuspended dust previously contaminated from irrigation water. This parameter is used by the GENII-S computer code (Leigh et al. 1993) to estimate the potential dose resulting from inhalation of radionuclides suspended in the air. To estimate inhalation exposure time, a time-activity budget was developed based on reasonable estimates of the behavior of people living in Amargosa Valley.
3. **Chronic Breathing Rate (m^3/day)** — Chronic breathing rate is the volume of air inhaled by a person per unit of time. This parameter is used to calculate the potential dose from inhaling contaminated dust particles. A literature review was conducted to identify the most appropriate value for this parameter.

The external exposure pathway evaluates potential radiation exposure from living and working in an environment (e.g., soil, vegetation) contaminated with radionuclides. External exposure is often referred to as groundshine. Three parameters for this pathway were analyzed in this report.

1. **Soil Exposure Time (hours/year)** — Soil exposure time is the amount of time a person spends outside in an area contaminated from groundwater irrigation. The time-activity budget developed for inhalation exposure time was used to estimate soil exposure time.
2. **Home Irrigation Rate (inches/year)** — Home irrigation rate is a measure of the amount of contaminated groundwater applied to the environment. This parameter is used to determine the level of contamination of the soil in the calculation of potential dose resulting from

groundshine. For this analysis, the irrigation requirements of locally grown turf grasses were calculated based on weather conditions in Amargosa Valley.

3. **Duration of Home Irrigation (months/year)** — Duration of home irrigation is the number of months during a year that groundwater is applied to the environment. This parameter is used to determine when a person may be exposed to soil that has been contaminated from groundwater irrigation. The irrigation requirements of locally grown turf grasses were considered to determine the value of this parameter.

Three estimates for each parameter were developed in this analysis. First, a distribution for each parameter was selected based on characteristics of the parameter or available data, and then reasonable, conservative estimates of the values were selected that define the distribution. Data distributions were selected from those that can be handled by the GENII-S computer code: fixed, normal, lognormal, triangular, uniform, loguniform, and empirical (Leigh et al. 1993, p. 5-33). Reasonable is defined as being reasonably expected to occur, based on (1) the characteristics of the critical group described in 10 CFR 63 regulations proposed by the Nuclear Regulatory Commission (NRC; 64 FR 8640-8678), (2) guidance from the Department of Energy (DOE) on the use of the proposed NRC regulations (Dyer 1999, p. 19 of Enclosure), and (3) information on the current population in Amargosa Valley (CRWMS M&O 1999d, pp. 22 and 23). Conservative is defined as a value or behavior that would result in a higher biosphere dose conversion factor. For example, watering a lawn for 12 months a year is considered more conservative than watering for fewer months because it would result in more frequent deposition of contaminated water and therefore a higher dose conversion factor. The second estimate for each parameter is a single, reasonably expected value to be used in a deterministic run of the GENII-S code, and was based on the type of distribution. The third estimate, to be used in an additional deterministic run of the GENII-S code, is a single, high bounding value that could occur based on extreme behaviors or conditions.

This analysis was conducted according to AP-3.10Q (Revision 1), *Analyses and Models*, and an approved development plan (CRWMS M&O 1999f). The only constraints, caveats, or limitations common to the entire analysis are those described above for reasonable/conservative and high bounding values.

All references cited in this document and listed in Section 8, other than those identified as inputs in Table 1, were included only to support or corroborate the assumptions, methods, and conclusion of the analyses and were not inputs required to produce the parameter values.

2. QUALITY ASSURANCE

The analyses in this AMR have been determined to be Quality Affecting in accordance with CRWMS M&O procedure QAP-2-0, *Conduct of Activities*, because the information will be used to support Performance Assessment and other quality-affecting activities. Therefore, this AMR is subject to the requirements of the *Quality Assurance Requirements and Description (QARD)* document (DOE 1998). This AMR is covered by the Activity Evaluation for *Scientific Investigation of Radiological Doses in the Biosphere* (CRWMS M&O 1999g).

Personnel performing work on this analysis were trained and qualified according to Office of Civilian Radioactive Waste Management (OCRWM) procedures AP-2.1Q, *Indoctrination and Training of Personnel*, and AP-2.2Q, *Establishment and Verification of Required Education and Experience of Personnel*. Preparation of this analysis did not require the classification of items in accordance with CRWMS M&O procedure QAP-2-3, *Classification of Permanent Items*. This analysis is not a field activity. Therefore, a *Determination of Importance Evaluation* in accordance with CRWMS M&O procedure NLP-2-0 was not required. The governing procedure for preparation of this AMR is OCRWM procedure AP-3.10Q, *Analyses and Models*.

3. COMPUTER SOFTWARE AND MODEL USAGE

No models were used or developed in this analysis. The only software used was an industry standard spreadsheet (Microsoft Excel). This spreadsheet was used as an aid in calculations; no routines, macros, or other applications were developed and used. Use of this software in this manner is exempt from the requirements in AP-SI.1Q, *Software Management*.

4. INPUTS

The inputs for each parameter are described and justified below and summarized in Table 1.

4.1 DATA

4.1.1 Mass Loading

Inhalable Particulate Matter (PM₁₀) (CRWMS M&O 1999b, parameter 1078). Twenty-four-hour measurements of particulate matter $\leq 10 \mu\text{m}$ (PM₁₀, $\mu\text{g}/\text{m}^3$) recorded at YMP Air Quality and Meteorological Monitoring Site 9 every six days from October 3, 1992 through December 30, 1997 were used to estimate this parameter. These data are summarized in CRWMS M&O (1999c, Table 2-3 on p. 13). Measurements of PM₁₀ were used for this analysis instead of total suspended particulates because the Environmental Protection Agency (EPA) National Ambient Air Quality Standards for particulate matter require the measurement of PM₁₀ (40 CFR 50.6, p. 7). In addition, PM₁₀ values were chosen because these sized particles are inhalable and can be deposited in the respiratory tract (EPA 1994b, Figure 3-3 on p. 3-10). Using PM₁₀ data for mass loading will result in a conservative estimate of resuspended radioactive particulate matter because it is unlikely that all resuspended particles will be contaminated. Airborne particulate matter is generated over a large up-wind area, and some of these areas will not be contaminated by irrigation water.

These data were selected because there was a reasonably large number of measurements (315 24-hour measurements taken over 5 years) collected close to the proposed location of the critical group using well documented, industry accepted methods. Site 9 is located near the southwest corner of the Nevada Test Site (CRWMS M&O 1999c, Figure 1-1 on p. 5 and Table 1-1 on p. 6), 3.1 km north of the proposed location of the critical group at the intersection of U.S. Highway 95 and Nevada Route 373 (Dyer 1999, p. 19 of Enclosure). Site 9 generally has southerly winds during the day and northerly winds at night (CRWMS M&O 1999c, Figure 3-5 on p. 3-7). Methods used to collect PM₁₀ data followed Nevada Work Instructions NWI-AQ-001, NWI-AQ-002, and NWI-AQ-016. The methods used to collect these data were based in part on 40 CFR

Table 1. Summary of inputs used in this analysis. See Sections 4.1.1 through 4.1.6 for justification of the use of these inputs.

Analysis Parameter	Input	TDMS Parameter Name (and Number)	Data Tracking Numbers or Citation	Qualification Status
Data				
Mass Loading	Inhalable particulate matter (PM ₁₀)	Particle Characteristics (1078)	MO98PSDALOG111.000 TM000000000001.039 TM000000000001.041 TM000000000001.042 TM000000000001.043 TM000000000001.079 TM000000000001.082 TM000000000001.084 TM000000000001.096 TM000000000001.097 TM000000000001.098 TM000000000001.099 TM000000000001.105 TM000000000001.108	TBV ^a TBV TBV TBV TBV TBV TBV TBV TBV TBV TBV TBV TBV TBV TBV
Home Irrigation Rate	Average monthly temperature	Temperature (595)	MO9903CLIMATOL.001	TBV ^b
Home Irrigation Rate	Average monthly solar radiation	Solar Flux (594)	MO9903CLIMATOL.001	TBV ^b
Home Irrigation Rate	Average monthly precipitation	Precipitation Quantity (553)	MO9903CLIMATOL.001	TBV ^b
Home Irrigation Rate	Crop coefficient (K _c):	NA	Devitt et al. (1992, Table 3 on p. 722; 1995b, Figure 2 on p. 56).	TBV ^c
Criteria				
All	Characteristics of the critical group	N/A	Dyer (1999, p. 19 of Enclosure); CRWMS M&O (1999d, pp. 22 and 23)	TBV ^d

^a Data need to be qualified.

^b Status of data qualification needs to be verified.

^c Source of data needs to be evaluated for classification as "accepted."

^d Analysis report (CRWMS M&O 1999d) needs to be completed.

50, Appendix J (pp. 65 through 70), and EPA Quality Assurance Handbook for Ambient Air Quality Monitoring (EPA 1994a, Section 2.11). The methods are described in CRWMS M&O (1997, p. 4) and earlier reports. The sample size is large enough that uncommon events such as very high winds that cause temporal variation in mass loading likely were sampled.

4.1.2 Inhalation Exposure Time

None.

4.1.3 Chronic Breathing Rate

None.

4.1.4 Soil Exposure Time

None.

4.1.5 Home Irrigation Rate

- 1. Average Monthly Temperature (°F) (CRWMS M&O 1999a, parameter 595).** Calculated from five years (1993–1997) of data collected at YMP Site 9. This site is at an elevation of 838 m (2,750 feet) (CRWMS M&O 1999c, Table 1-1 on p. 6), near the southwest corner of the Nevada Test Site and 3.1 km north of the proposed location of the critical group at the intersection of U.S. Highway 95 and Nevada Route 373 (Dyer 1999, p. 19 of Enclosure).

These data were selected because this weather station is the closest station to the proposed location of the critical group and the data were collected under a YMP program that met the requirements of the QARD (DOE 1998). The data are presented in CRWMS M&O (1999c, Table A-9 on p. A-10). For use in the Jensen-Haise equation (see Appendix A), temperatures were converted from the measured units of degrees celsius (°C) to degrees fahrenheit (°F) using the equation $^{\circ}\text{F} = (9/5\ ^{\circ}\text{C}) + 32$.

- 2. Average Daily Incoming Solar Radiation Per Month (langleys/day) (CRWMS M&O 1999a, parameter 594).** Calculated from five years of data collected at YMP Site 9. These data were selected because this weather station is the closest station to the proposed location of the critical group (Dyer 1999, p. 19 of Enclosure) and the data were collected under a YMP program that met the requirements of the QARD (DOE 1998). The data are presented in CRWMS M&O (1999c, Table A-9 on p. A-10). For the calculation of evapotranspiration (ET), the data were converted from the measured units of megajoules/m²/day to langleys/day using the equation $\text{langleys/day} = 23.89 (\text{megajoules/m}^2/\text{day})$.
- 3. Average Annual Precipitation (CRWMS M&O 1999a, parameter 553).** Calculated from five years of data collected at YMP Site 9. These data were selected because they were collected under a YMP program that met the requirements of the QARD (DOE 1998) and the weather station is the closest station to the proposed location of the critical group (Dyer 1999, p. 19 of Enclosure). The data are presented in CRWMS M&O (1999c, Table A-9 on p. A-10).
- 4. Crop Coefficient (K_c)** Monthly crop coefficients for bermudagrass and tall fescue are as reported in Devitt et al. (1992, Table 3 on p. 722; 1995b, Figure 2 on p. 56). These values are summarized in Table 3 in Section 6.4.

Crop coefficient is an expression of the ET of a plant species relative to the potential ET of a reference species. Crop coefficients are commonly used in calculations of ET because field measurements of potential ET for an area only are needed for one reference crop (Martin et al. 1991a, p. 201).

The crop coefficients for low maintenance bermudagrass (Devitt et al. 1992, Table 3 on p. 722) and tall fescue (Devitt et al. 1995b, Figure 2 on p. 56) were obtained from studies of bermudagrass ET conducted in Las Vegas, Nevada. These values were selected because they come from peer-reviewed, published studies conducted closer to Yucca Mountain than any other published values (e.g., Devitt et al. 1995a, Table 2 on p. 68). The studies were conducted using widely accepted methods for measuring ET by scientists that have experience using these methods.

These coefficients were developed using a reference crop of cool-season grass, whereas the Jensen-Haise ET equation used in this analysis is for a reference crop of alfalfa. UCCE (1987, p. 6) state that "Several agencies and researchers have recommended using ET_o [i.e., from grass] directly as a method to estimate alfalfa ET_c [i.e., crop coefficient for alfalfa]." Conversely, Martin et al. (1991a, p. 202) state that grass usually uses 10-15% less water than alfalfa; thus, using a grass-based coefficient with an alfalfa-based estimate of ET may result in an 10-15% overestimate of water requirements. Therefore, this is an acceptable, conservative input for this analysis.

4.1.6 Duration of Home Irrigation

None.

4.2 CRITERIA

For all analyses, assumptions about the characteristics of the critical group were based on DOE interim guidance (Dyer 1999, p. 19 of Enclosure) on rules proposed by the NRC for 10 CFR 63, Section 115 (64 FR 8640-8678). In addition, a more detailed description of the critical group (CRWMS M&O 1999d, pp. 22-23) based on DOE guidance, a survey of people in Amargosa Valley, and U.S. Bureau of the Census data for the Amargosa Valley Census County Division, also was considered during the analysis of all parameters.

4.3 CODES AND STANDARDS

None.

5. ASSUMPTIONS

5.1 Mass Loading

None.

5.2 Inhalation Exposure Time

Three assumptions about the behavior of members of the critical group were made for the analysis of inhalation exposure time.

1. When in a contaminated area, the exposure rate experienced while indoors (including time spent inside vehicles) is half of that experienced while outdoors. This assumption is based on shielding factors recommended by the NRC (1977, p. 1.109-43). Because this shielding factor was developed by the regulatory agency responsible for licensing a repository at Yucca Mountain, this assumption does not need to be confirmed.
2. The average member of the critical group spends a certain amount of time each day outdoors tending a garden plot and doing other activities. Time spent outdoors by the average member of the critical group was assumed to be 827 hours/year (EPA 1997b, Table 15-120 on p. 15-136). This value is the amount of time "spent at home in the yard or other areas outside the home" based on survey data from 1301 adults, 18 years or older. The value of 827 hours/year is more conservative and more age-specific than 548 hours/year from a California study of 1,762 people 12 years of age or older (EPA 1997b, Table 15-7 on p. 15-25) or 450 hours/year from a nationwide survey of 2,762 people 12 years of age or older (EPA 1997b, Table 15-7 on p. 15-25). Therefore, 827 hours is a valid assumption of the time spent outdoors by adults and does not need to be confirmed.
3. Three lifestyle scenarios resulting in different inhalation exposure times were assumed to bound the distribution:
 - *Average*—The average member of the critical group is employed 35 hours/week, 50 weeks/year, in the vicinity of Yucca Mountain in a non-farming occupation. This is 1,750 hours/year (where one year equals 8,760 hours). This assumption is based on characteristics of the critical group described in CRWMS M&O (1999d, p. 23). Commuting time to and from work is within the contaminated area and is assumed to be 5 minutes (0.083 hour) in each direction based on the U.S. Bureau of the Census data estimate of the modal (the most frequently reported) commuting time for the area (CRWMS M&O 1999d, p. 22).
 - *Least Exposed*—This person works indoors or outdoors the same number of hours as the average member of the group, and the work locality is in a non-contaminated area. Commuting time to and from work is considered to take place in a non-contaminated area. Commuting time was assumed to be 0.5 hour based on U.S. Bureau of the Census data on median (the value that divides a frequency distribution into two halves) commuting time for the area (CRWMS M&O 1999d, p. 22). The least exposed person has a sedentary lifestyle and spends little time outdoors (25% of that determined for the average person).
 - *Most Exposed*—This person works outdoors 60 hour/week (12 hours/day, 5 days/week; 3,120 hours/year) in a contaminated area (e.g., an irrigated agricultural area). Commuting time to and from work is within the contaminated area and is assumed to be 5 minutes (0.083 hour) in each direction based on the U.S. Bureau of the Census data

estimate of the modal (the most frequently reported) commuting time for the area (CRWMS M&O 1999d, p. 22). In addition, this person spends additional time outdoors tending a garden at home (the same amount as the average member of the group). This scenario is intended to be similar to the lifestyle of an agricultural worker, of which there are relatively few (< 3% of the population) in Amargosa Valley (CRWMS M&O 1999d, p. 22).

These assumptions are based on DOE interim guidance (Dyer 1999, pp. 19 of Enclosure), CRWMS M&O (1999d, pp. 22 and 23), and reasonable estimates of the behavior of people in Amargosa Valley, and therefore do not need to be confirmed.

5.3 Chronic Breathing Rate

None.

5.4 Soil Exposure Time

The same assumptions about behaviors of the critical group developed for inhalation exposure time (Section 5.2) were made for the analysis of soil exposure time.

5.5 Home Irrigation Rate

1. Deep percolation is the amount of water that passes below the root zone. In mesic regions, deep percolation can result from precipitation or irrigation in excess of ET that percolates beyond the root zone. In arid agricultural systems, deep percolation occurs intentionally during irrigation to leach salts (i.e., flush them below the root zone) that are deposited in the soil from irrigation water and that would decrease plant production. The most accurate way to measure deep percolation is to install underground lysimeters, which measure the amount of water that moves below the root zone (e.g., Devitt et al. 1992, pp. 717 through 723). Review of published literature and discussions with University of Nevada Cooperative Extension personnel indicated that no lysimeter measurements have been performed in the agricultural areas surrounding Yucca Mountain.

In the absence of site specific data, a value of six inches was assumed for this analysis. This value was selected to be consistent with the value of percolation implied in the GENII-S code and to be compatible with other portions of that code (Napier et al. 1988, p. 4.58). The validity of this value for irrigation of tall fescue in Amargosa Valley, which is less salt-tolerant than bermudagrass (Martin et al. 1991a, Table 10-10 on p. 223), was checked using two equations, as shown in Appendix B. These equations use information on salt content of irrigation water and salt tolerance of plants to determine the amount of water required to leach salts. Values of 0.9 and 3.3 inches were calculated (Appendix B), which are substantially below the default value of 6 inches. Based on these calculations, deep percolation of 6 inches is considered a valid assumption for this analysis, and does not need to be confirmed

2. The high bounding value for irrigation rate is 25% higher than the irrigation requirement for tall fescue. Irrigation rates higher than actual requirements would result from such factors as

inefficient irrigation systems, intentional or unintentional over-irrigating, and higher leaching requirements on soils with high salt content. Although rates greater than 25% are possible, it is unlikely that someone would reach such an extreme because of the increased cost for pumping or buying groundwater and the detrimental effects that such high levels of overwatering would have on turfgrass and the rest of their landscape. No data are available to confirm this assumption.

5.6 Duration of Home Irrigation

None.

6. ANALYSIS

6.1 MASS LOADING

One input, PM₁₀ data from YMP Site 9 (Section 4.1.1), and no assumptions were used in the analysis of mass loading.

The reasonable, conservative distribution of mass loading was determined directly from the Site 9 PM₁₀ data. Distributions that can be handled by the GENII-S computer code include fixed, normal, lognormal, triangular, uniform, loguniform, and empirical (Leigh et al. 1993, p. 5-33). The raw PM₁₀ data were skewed toward low values (Figure 1) and a logarithmic transformation (log base 10) resulted in the best fit to the available distributions (Figure 2). Two zero values were removed from the data set prior to transformation because the logarithm of zero is an undefined value. Because the empirical distribution in GENII-S (which samples the data points to obtain a value each time during a run of the program) is restricted to only 100 data points (Leigh et al. 1993, p. 5-36) and the PM₁₀ data set was much larger, lognormal was chosen as the best distribution for PM₁₀ data.

GENII-S requires two values to define a lognormal distribution, the 0.1 (minimum) and 99.9th (maximum) percentiles. These percentiles were calculated using the mean and standard deviation of the log transformed data and the Z-distribution, using the equations:

$$\text{Minimum} = \mu - Z\sigma, \text{ and}$$

$$\text{Maximum} = \mu + Z\sigma,$$

where μ and σ are the mean (0.838) and standard deviation (0.313), respectively, of the log transformed PM₁₀ data, and Z (3.09) is the value that describes the proportion of the normal curve that lies

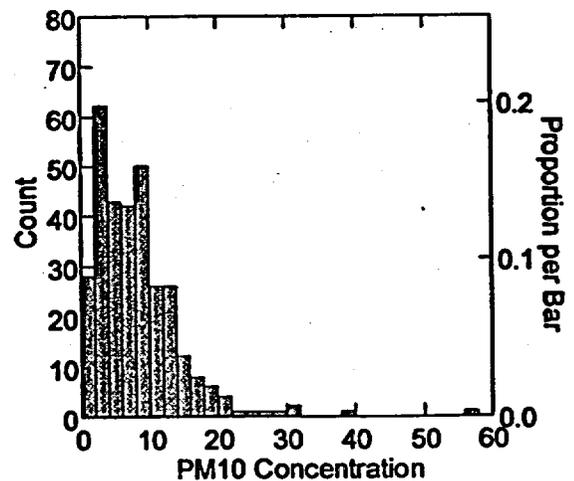


Figure 1. Untransformed PM₁₀ concentration data (µg/m³) from Site 9, 10/3/92 to 12/30/97 (CRWMS M&O 1999b).

beyond a given normal deviate. These calculations resulted in a minimum log-transformed value of -0.1292 and a maximum log-transformed value of 1.805. Back calculating these values (i.e., taking the antilog) resulted in a minimum value of 0.743 $\mu\text{g}/\text{m}^3$ and a maximum value of 63.836 $\mu\text{g}/\text{m}^3$.

The mean of the non-transformed data, 8.725 $\mu\text{g}/\text{m}^3$, was selected as the reasonably expected estimate for a deterministic run.

The PM₁₀ 99.9th percentile value described by the distribution (63.86 $\mu\text{g}/\text{m}^3$) was selected as the high bounding value because it is about 12% higher than the highest PM₁₀ value (57 $\mu\text{g}/\text{m}^3$) recorded at Site 9.

PM₁₀ data were recorded in $\mu\text{g}/\text{m}^3$ and converted to units of g/m^3 (values usable by GENII-S) by multiplying by 1.0×10^{-6} . The resulting estimates were a minimum of $7.4 \times 10^{-7} \text{ g}/\text{m}^3$ and a maximum of $6.4 \times 10^{-5} \text{ g}/\text{m}^3$. The reasonable expected value was 8.7×10^{-6} and the high bounding value was $6.4 \times 10^{-5} \text{ g}/\text{m}^3$.

6.2 INHALATION EXPOSURE TIME

Based on the three assumptions listed in Section 5.2, a time activity budget was developed for the three lifestyle scenarios (Table 2). The inhalation exposure time category in Table 2 is the amount of time in hours per year that a member of the critical group is assumed to be exposed to, and will be inhaling, aerosolized radioactive material (i.e., dust). Inhalation exposure time (IET) is calculated using the equation:

$$IET = T_{OC} + \frac{T_{IC}}{2},$$

where T_{OC} equals the time spent outdoors in a contaminated area, and T_{IC} equals the number of hours spent indoors in a contaminated area. This equation is based on the assumption (#1 in Section 5.2) that the exposure rate indoors is one-half of that experienced outdoors.

The reasonable, conservative distribution of inhalation exposure time has a triangular probability function. The number of hours assumed to be spent outdoors by the most exposed individual is much higher than that of the average individual; therefore, symmetrical distributions (e.g., normal and uniform) are not valid. The triangular distribution was chosen because there is no information to indicate that more complex non-symmetrical distributions are more likely than the triangular distribution. This triangular distribution is described by a minimum value of 3,483.38 hours/year, the mode (referred to as best estimate in GENII-S, Leigh et al. 1993, p. 5-33) of 3,918.5 hours/year, and a maximum of 6,353.5 hours/year (Table 2). The reasonably expected value to use in a deterministic run of the GENII-S code is the mode of 3,918.5 hours/year.

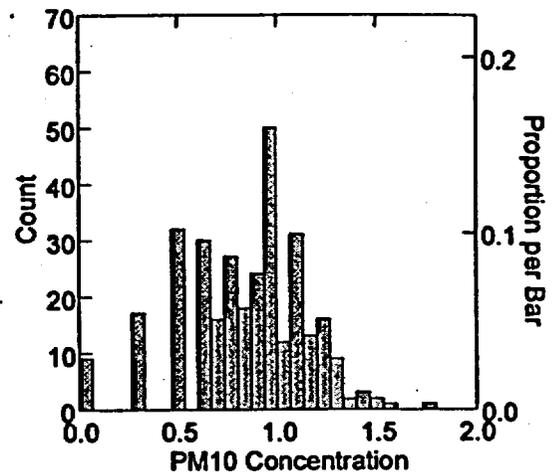


Figure 2. Log (base 10) transformed PM₁₀ concentration data ($\mu\text{g}/\text{m}^3$) from Site 9, 10/3/92 to 12/30/97 (CRWMS M&O 1999b).

Table 2. Time (hours/year) spent in contaminated and uncontaminated areas based on three lifestyle scenarios.

Scenario	Activity	Contaminated Areas		Non-contaminated Areas		Inhalation Exposure Time ^a
		Outdoors	Indoors	Outdoors plus Indoors		
Least Exposed	At work	0.00	0.00	1750.00		
	Commuting	0.00	0.00	250.00		
	At home	206.75	6553.25	0.00		
	Total	206.75	6553.25	2000.00		3483.38
Average	At work	0.00	0.00	1750.00		
	Commuting	0.00	41.50	0.00		
	At home	827.00	6141.50	0.00		
	Total	827.00	6183.00	1750.00		3918.50
Most Exposed	At work	3120.00	0.00	0.00		
	Commuting	0.00	43.00	0.00		
	At home	827.00	4770.00	0.00		
	Total	3947.00	4813.00	0.00		6353.50

^a Calculated as 100% of time spent outdoors in a contaminated area plus 50% of time spent indoors in a contaminated area (NRC 1977, p. 1.109-43).

The maximum estimate was also selected as the high bounding value. This maximum estimate was based on the lifestyle (i.e., outdoor worker such as a farmer working in the contaminated area) that will result in a high exposure rate relative to the average member of the critical group. The number of hours that this worker is assumed to spend outdoors (working 60 hours/week for 52 weeks, plus 827 additional hours spent outdoors, totaling 3,947 hours/year) is higher than the values from two other recent studies. The NRC, in their Iterative Performance Assessment Phase 2 (NRC 1995, p. 7-10), used a lower value by assuming that farmers spent only 27% of their time outdoors (6.48 hours/day or 2,336 hours/year), resulting in an inhalation exposure time of 5,548 hours/year. In addition, LaPlante and Poor (1997, p. 2-23) assumed that time spent outdoors for a "resident farmer" who was employed outside of the contaminated area (2,080 hours/year) would equal 100 hours/year in a garden and 1,700 additional hours outdoors. This scenario results in an inhalation exposure time of 4,200 hours/year (LaPlante and Poor 1997, p. 2-23).

6.3 CHRONIC BREATHING RATE

Estimates of chronic breathing rates were selected based on a literature review of the breathing rates of adults. Only adults were considered because DOE interim guidance (Dyer 1999, p. 19 of Enclosure) and proposed NRC guidelines (64 FR 8677) state that the average member of the critical group is an adult.

Several breathing rates have been used to assess exposure to airborne contaminants (reviewed in EPA 1997a, pp. 5-1 through 5-27). The following are examples of the range of values previously used and include the estimates chosen for the chronic breathing rate parameter.

- The EPA *Exposure Factors Handbook* recommends a value of 15.2 m³/day for an adult male, 19 to 65 years of age (reviewed in EPA 1997a, p. 5-24). However, EPA (1997a, p. 5-1) states that a value of 20 m³/day is used as the default value for the EPA *Integrated Risk Information System*.
- The International Commission on Radiological Protection (ICRP), Publication 23 (ICRP 1975, p. 346), uses a value of 23 m³/day for a 70-kg adult male. This value is based on eight hours each of resting, light activity work, and nonoccupational activity.
- ICRP (1975, p. 346) also identifies a value of 31 m³/day (i.e., 35% more than the 23 m³/day for an average lifestyle) for a 70-kg adult male that is engaged in more strenuous activities.
- Based on the information in ICRP (1975, pp. 346 and 347), an adult male engaging in moderate to heavy activity for 16 hours/day and resting for 8 hours/day would consume approximately 42 m³/day.

Chronic breathing rate was considered to have a fixed distribution because the GENII-S code treats this input as a fixed value. The ICRP value of 23 m³/day was selected as the reasonable, conservative estimate and as the reasonably expected value to use in a deterministic run of GENII-S. This value was selected primarily because it is based on a scenario that matches the behavioral characteristics of the reference group as proposed by the NRC (64 FR 8640-8678) and described in CRWMS M&O (1999d, pp. 22 and 23). In addition, ICRP (1975) is considered the international standard for physical and physiological characteristics of "reference man."

The ICRP value of 31 m³/day was selected as the high bounding value because it matches a likely scenario for a person in Amargosa Valley working outdoors in an agricultural setting. The high value of 42 m³/day was considered unreasonable because it is doubtful that a person could sustain the level of activity required to maintain this high breathing rate.

6.4 SOIL EXPOSURE TIME

The assumptions, scenarios, and much of the analyses for determining soil exposure time are the same as those for determining inhalation exposure time (see Section 6.2), and are not repeated here. The only difference between these parameters is that inhalation exposure time includes time spent indoors in a contaminated environment; soil exposure time does not. Thus, the values presented in Table 2 for time spent outdoors in a contaminated environment are equal to the soil exposure time.

Based on the information presented in Section 6.2, the reasonable, conservative distribution of soil exposure time is triangular with a minimum estimate of 206.75 hours/year, the mode (referred to as best estimate in GENII-S, Leigh et al. 1993, p. 5-33) of 827.0 hours/year, and maximum estimate of 3,947.0 hours/year. The reasonably expected value to use in a

deterministic run of GENII-S is the mode of 827.0 hours/year. The high bounding value is the maximum value of 3,947.0 hours/year.

6.5 HOME IRRIGATION RATE

The irrigation rate of turfgrass was calculated for this analysis. Turf was chosen because lawns are common in southern Nevada, turf requires year-round irrigation in this region, and turf has a high water requirement relative to garden crops and ornamental plants; thus, it will result in a realistic and conservative estimate of home irrigation rate. The data listed in Section 4.1.5 were used as inputs for temperature, solar radiation, precipitation, and crop coefficients. Assumptions were developed for deep percolation and the high bounding value (Section 5.5).

Irrigation rate of turfgrass is influenced by the type of grass grown and the maintenance regime followed (Devitt et al. 1992, pp. 717 through 723). Two combinations of turf and maintenance regimes were analyzed to obtain a range of home irrigation rates. For a low estimate, irrigation rate was calculated for warm-season bermudagrass overseeded with perennial ryegrass during winter and grown in a low-maintenance (e.g., low rate of fertilizer application, low mowing frequency, high mowing height) park setting, as described by Devitt et al. (1992, pp. 717 through 723). For a high estimate, irrigation rate was calculated for cool-season tall fescue grass grown under a relatively high-maintenance regime as described by Devitt et al. (1995b, pp. 47 through 63).

Irrigation requirements for low-maintenance bermudagrass and high-maintenance tall fescue represent a reasonable, conservative range of irrigation rates for turfgrass in southern Nevada. Bermudagrass is a commonly used, drought adapted turfgrass in southern Nevada (Morris and Johnson 1991, p. 1). Although maintenance regimes resulting in lower irrigation rates often are used in southern Nevada (e.g., no winter overseeding or irrigation, and allowing grass to die back during mid-summer), the park-based maintenance regime used in this analysis will result in a higher, more conservative estimate. The irrigation rate of tall fescue is suitable for the high estimate because cool season grasses are not as well adapted to arid climates as warm-season grasses and require about 20-30% more irrigation water (Morris and Johnson 1986, pp. 1 through 3; Undated B, p. 1), and because tall fescue is the recommended cool season grass for southern Nevada (Morris and Johnson, 1986, p. 3).

Irrigation rate (IR, inches/year) was calculated using the equation:

$$IR = \sum_{m=1}^{12} ET_m - P + DP,$$

where m = month, ET_m = total monthly ET, P = annual precipitation, and DP = annual deep percolation. This equation is a reduction of the soil water balance equation in Martin et al. (1991a, p. 200), based on a steady-state condition (i.e., soil water at the beginning of the year equals that at the end of the year). This equation accounts for the water needs of the plant being irrigated (transpiration) and the major site-specific inputs (precipitation and deep percolation) and outputs (evaporation) of water.

Evapotranspiration for a plant species typically is calculated based on the ET for a reference crop (i.e., reference ET) at the location of interest multiplied by a coefficient specific to the species being considered (Martin et al. 1991a, pp. 201 through 204; UCCE 1987, pp. 1 through 12). For this analysis, reference ET was calculated using the Jensen-Haise equation (Martin et al. 1991b, p. 334), as described and justified in Appendix A and summarized in Table 3.

Monthly ET was calculated by multiplying reference ET by the monthly crop coefficients for bermudagrass (Devitt et al. 1992, Table 3 on p. 722) and tall fescue (Devitt et al. 1995b, Figure 2, on p. 56). Monthly ET for bermudagrass ranged from 0.84 inches in December and January to 8.26 inches in July and totaled 49.2 inches annually (Table 3). Actual annual ET of low-maintenance bermudagrass in Las Vegas has been measured at 42 inches (Devitt et al. 1992, p. 720). Monthly ET for tall fescue ranged from 0.65 inches in December to 15.32 inches in July, and totaled 84.5 inches annually (Table 3). Actual annual ET of tall fescue in Las Vegas has been measured at 87 inches (Devitt et al. 1995b, p. 59).

Using values of 3.59 inches annual precipitation and 6 inches deep percolation, the minimum irrigation rate (inches/year), based on the requirements of low-maintenance bermudagrass, is

$$IR = \sum_{m=1}^{12} ET_m - P + DP = 49.2 - 3.6 + 6 = 51.6.$$

This value is slightly lower than the estimate of about 60 inches/year for the Las Vegas Valley (Morris and Johnson 1991, p. 3). It is also lower than the rate of 74 inches/year recommended for bermudagrass by the Las Vegas Valley Water District (Undated, pp. 10 and 11). It is expected that these published estimates are somewhat higher than the estimate calculated for this analysis because the published estimates are based on a high-maintenance regime. They also use a higher deep percolation rate (15% of annual irrigation = 9 or 13 inches, respectively) because of the high salinity of the Colorado River water used in Las Vegas (Las Vegas Valley Water District Undated, pp. 10 and 11). Thus, a rounded estimate of 52 inches/year based on site-specific information is a valid estimate of the minimum irrigation rate used by a member of the critical group.

The maximum irrigation rate (inches/year), based on the requirements of tall fescue, is

$$IR = \sum_{m=1}^{12} ET_m - P + DP = 84.5 - 3.6 + 6 = 86.9.$$

This value is slightly lower than 91 inches/year recommended for tall fescue by the Las Vegas Valley Water District (Undated, pp. 12 and 13). However, it is similar after differences in deep percolation are accounted for (about 12 inches in Las Vegas versus 6 inches for this analysis). Thus, 87 inches/year is a valid estimate of the maximum irrigation rate used by a member of the critical group.

Table 3. Average monthly temperature and solar radiation at YMP Site 9, monthly reference evapotranspiration (ET_r), and monthly crop coefficients and evapotranspiration for bermudagrass and tall fescue. Values presented are rounded. Calculations were done using more precise values from the original data sources.

Month	Average Monthly Temperature		Average Daily Solar Radiation		ET _r (Inches) ^d	Crop Coefficient		Evapotranspiration (Inches) ^e	
	°C ^a	°F ^b	mJ/m ² /day ^a	langleys/day ^c		Bermudagrass ^e	Tall Fescue ^f	Bermudagrass	Tall Fescue
January	7.1	44.8	9.5	227.0	2.04	0.41	0.54	0.84	1.10
February	9.6	49.3	13.9	332.1	3.09	0.41	0.72	1.27	2.22
March	13.6	56.5	19.4	463.5	5.73	0.41	0.86	2.35	4.93
April	16.7	62.1	24.6	587.7	7.95	0.55	0.96	4.37	7.63
May	22.1	71.8	27.5	657.0	11.02	0.55	1.02	6.06	11.24
June	27.4	81.3	29.9	714.3	13.49	0.55	1.04	7.42	14.03
July	31.0	87.8	29.4	702.4	15.02	0.55	1.02	8.26	15.32
August	30.5	86.9	27.0	645.0	13.63	0.55	0.96	7.49	13.08
September	25.4	77.7	22.6	539.9	9.66	0.55	0.86	5.31	8.31
October	17.7	63.9	17.4	415.7	6.03	0.55	0.72	3.31	4.34
November	10.6	51.1	11.9	284.3	2.98	0.55	0.54	1.64	1.61
December	6.9	44.4	9.6	229.3	2.04	0.41	0.32	0.84	0.65
Annual Sum					92.69			49.17	84.48

^a CRWMS M&O 1999a.

^b Converted as $(9/5)°C+32$.

^c Converted as langleys/day = 23.89(megajoules/m²/day).

^d See Appendix A for details about the calculation of reference evapotranspiration.

^e Average of five years of experimental data with months grouped to maximize uniformity coefficients (Devitt et al. 1992, pp. 721 and 722).

^f Calculated from the equation: Crop Coefficient = $0.32 + 0.24(\text{month}) - 0.02(\text{month})^2$, where month is a numeric value for the order of months in a year (e.g., February = 2) (Devitt et al. 1995b, Figure 2).

^g Evapotranspiration = ET_r × crop coefficient.

The reasonable, conservative distribution of home irrigation rate has a uniform probability function. The actual rate at which turfgrass is irrigated is dependent upon numerous decisions made by the residents, such as fertilization rates, frequency of mowing, and the efficiency of irrigation equipment. These choices are dependent upon the quality of grass residents desire and the amount of effort and money they are willing to expend on maintaining their lawn. Because the range of these choices is based on personal preference, and all choices are equally likely, a uniform distribution was selected.

Based on this analysis, the reasonable, conservative distribution of home irrigation rate has a uniform probability distribution with a minimum of 52 inches/year and a maximum of 87 inches/year. The reasonably expected value to be used in a deterministic run of GENII-S is 69.5 inches/year, the midpoint between the minimum and maximum values. Based on Assumption 2 in Section 5.5, the high bounding value is 109 inches/year (25% greater than the maximum of the distribution).

6.6 DURATION OF HOME IRRIGATION

For the reasons described in the analysis of home irrigation rate (Section 6.5), the irrigation requirements of turfgrass were considered in this analysis. A literature review was conducted to determine the irrigation requirements of turfgrass species.

The Las Vegas Valley Water District (Undated, pp. 10 through 13) and the University of Nevada Cooperative Extension (Morris and Johnson 1991, pp. 3 and 4; Morris and Van Dam 1989, pp. 3 and 4) recommend that cool and warm season grasses be irrigated throughout the year in southern Nevada.

Based on these recommendations, the reasonable, conservative distribution is a fixed value of 12 months. The reasonably expected and high bounding values to be used in deterministic runs of GENII-S also are the maximum possible value of 12 months.

7. CONCLUSIONS

This analysis report documents the selection of the recommended reasonable, conservative distribution; reasonably expected value; and high bounding value for six parameters needed to calculate biosphere dose conversion factors (Table 4).

The primary uncertainty associated with these recommendations is the definition and characteristics of the critical group, which are defined in DOE guidance (Dyer 1999, p. 19 of Enclosure) and summarized in CRWMS M&O (1999d, pp. 22 and 23). These characteristics are based on rules proposed by the NRC for 10 CFR 63 (64 FR 8640-8678). If the final NRC rules differ from the proposed rules enough to cause changes in DOE guidance or the characteristics summarized in CRWMS M&O (1999d, pp. 22 and 23), revision of this analysis will have to be considered. Similarly, if CRWMS M&O (1999d, pp. 22 and 23), which is classified as To Be Verified (TBV) (Table 1 and Attachment 1), is modified during the review process, this analysis may have to be modified.

Table 4. Summary of parameter values for GENII-S code input derived from analyses presented in this report.

Pathway Parameter	Distribution	Reasonably Expected Value ^a	High Bounding Value ^a
Exposure from Inhalation			
Mass Loading (grams/m ³)	Lognormal: 0.1 percentile = 7.4×10^{-7} , 99.9 percentile = 6.4×10^{-5}	8.7×10^{-6}	6.4×10^{-5}
Inhalation Exposure Time (hours/year)	Triangular: min = 3,483.38, mode ^b = 3,918.5, max = 6,353.5	3,918.5	6,353.5
Chronic Breathing Rate (m ³ /day)	Fixed: 23	23	31
External Ground Exposure			
Soil Exposure Time (hours/year)	Triangular: min = 206.75, mode ^b = 827, max = 3,947	827	3,947
Home Irrigation Rate (inches/year)	Uniform: min = 52, max = 87	69.5	109
Duration of Home Irrigation (months/year)	Fixed: 12	12	12

^a These values are estimates required for deterministic runs of the computer model, GENII-S.

^b Referred to as the best estimate in GENII-S (Leigh et al. 1993, p. 5-33).

Five other inputs for this analysis are classified as TBV (Table 1 and Attachment 1). If these inputs, listed below, are not verified, assumptions will have to be developed to replace those inputs. It is likely that those assumptions will be based on the same data now used as inputs, and therefore the results of the analysis will not change. However, confidence in the conclusions of this analysis may be less if based on unverified assumptions.

- The data used to estimate mass loading (CRWMS M&O 1999b, parameter 1078) needs to be evaluated for qualification as described in AP-SIII.2Q, *Qualification of Unqualified Data and the Documentation of Rationale for Accepted Data*. This process has been initiated.
- The qualification status of three inputs in the analysis of home irrigation rate needs to be verified. These inputs are average monthly temperature, solar radiation and precipitation (parameters 595, 594, and 553, respectively, in CRWMS M&O 1999a). A TBV number has been assigned and this process, as defined in AP-3.15Q, *Managing Technical Product Inputs*, has been initiated.
- The source (University of Nevada Cooperative Extension) for the crop coefficients of turf grasses used in the analysis of home irrigation rates needs to be evaluated for classification as accepted, as described in AP-SIII.2Q. This process has been initiated.

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8.3 CODES, STANDARDS, AND REGULATIONS

40 CFR 50, Appendix J (1996). Reference Method for the Determination of Particulate Matter as PM₁₀ in the Atmosphere.

40 CFR 50.6 (1996). Primary and Secondary Ambient Air Quality Standards for PM₁₀.

64 FR 8640-8678 (1999). Disposal of High-Level Radioactive Wastes in a Proposed Geologic Repository at Yucca Mountain, Nevada.

8.4 PROCEDURES

AP-2.1Q, *Indoctrination and Training of Personnel*

AP-2.2Q, *Establishment and Verification of Required Education and Experience of Personnel*

AP-3.10Q, *Analyses and Models*

AP-3.15Q, *Managing Technical Product Inputs*

AP-SI.1Q, *Software Management*

AP-SIII.2Q, *Qualification of Unqualified Data and the Documentation of Rationale for Accepted Data*

NLP-2-0, *Determination of Importance Evaluations*

NWI-AQ-001 (Nevada Work Instruction AQ-001) 1995a. *Routine Operations and Maintenance for Ambient Particulate Matter Sampling*. Las Vegas, Nevada.

NWI-AQ-002 (Nevada Work Instruction AQ-002) 1995b. *Calibrations and Performance Audits of Particulate Matter Samplers*. Las Vegas, Nevada.

NWI-AQ-016 (Nevada Work Instruction AQ-016) 1995c. *Air Quality Monitoring: Gaseous and Particulate Data Processing Instructions*. Las Vegas, Nevada.

QAP-2-0, *Conduct of Activities*

QAP-2-3, *Classification of Permanent Items*

APPENDIX A

**CALCULATION OF REFERENCE EVAPOTRANSPIRATION (ET_R)
AND JUSTIFICATION OF THE SELECTED EQUATION.**

**APPENDIX A. CALCULATION OF REFERENCE EVAPOTRANSPIRATION
(ET_r) AND JUSTIFICATION OF THE SELECTED EQUATION.**

Calculation

Monthly reference evapotranspiration was calculated using the Jensen-Haise equation (Martin et al. 1991b, p. 334):

$$ET_r = \frac{C_T(T - T_x)R_s}{1486} \text{ days}$$

where:

$$C_T = 1/(C_1 + C_2C_H) = 1/\{58.10 + 13(1.11)\} = 0.014$$

$$C_1 = 68 - 3.6(\text{elevation in feet})/1,000 = 68 - 3.6(2,750)/1,000 = 58.10$$

$$C_2 = 13, \text{ }^\circ\text{F (a constant)}$$

$$C_H = 50/(e_2 - e_1), \text{ mbars} = 50/(70.74 - 25.63) = 1.11$$

$$T_x = 27.5 - 0.25(e_2 - e_1) - \text{elevation}/1,000 = 27.5 - 0.25(70.74 - 25.63) - 2,750/1,000 = 13.47$$

e_2 = saturated vapor pressure (mbars) at the mean maximum air temperature for the hottest month (39.2°C; CRWMS M&O 1999a; CRWMS M&O 1999c, Table A-9 on p. A-10). Calculated using the following equation from Buck (1981, p. 1532):

$$e_s = 6.1121 \left\{ \exp \left(\frac{17.502(^\circ\text{C})}{(240.97 + ^\circ\text{C})} \right) \right\} = 6.1121 \{ \exp(2.45) \} = 70.74$$

e_1 = Saturated vapor pressure (mbars) at the mean minimum air temperature for the hottest month (21.5°C; CRWMS M&O 1999a; CRWMS M&O 1999c, Table A-9 on p. A-10). Calculated using the following equation from Buck (1981, p. 1532):

$$e_s = 6.1121 \left\{ \exp \left(\frac{17.502(^\circ\text{C})}{(240.97 + ^\circ\text{C})} \right) \right\} = 6.1121 \{ \exp(1.43) \} = 25.63$$

R_s = Incoming solar radiation, langley/day (See Table 3)

T = Average monthly air temperature, °F (See Table 3)

days = number of days per month

Example: (average monthly temperature and solar radiation are from Table 3)

January ET_r (inches) =

$$ET_r = \frac{0.014(44.8 - 13.47)227}{1486} 31 = 2.04.$$

Justification of Jensen-Haise Equation:

The Jensen-Haise equation was chosen for the calculation of reference ET because it is relatively simple to use and is generally reliable for calculating ET over long periods (e.g., weekly) in arid climates using the type of climate data available for the Amargosa Valley region (Martin et al. 1991b, p. 334). This equation accounts for local temperature and solar radiation. However, it does not incorporate the effects of wind, as do more complicated methods such as the modified Penman equation (Martin et al. 1991b, pp. 334 through 336). Devitt et al. (1995a, pp. 75 through 81) demonstrated that high wind runs can influence calculations of ET in the southwestern United States.

To ensure that the Jensen-Haise equation did not underestimate reference ET, the results calculated for this analysis (Table 3) were compared to two unpublished estimates of ET for southern Nevada that used the modified-Penman equation (Figure A-1). The first was calculated from nine years (1986–1994) of climate data from Pahrump, Nevada (Contact Report; S.L. LeStrange to G.D. McCurdy, Western Regional Climate Center, Reno Nevada; including computer code, weather data, and results of equation; ACC: MOL.19990323.0175). The second was based on four years of data (1988, 1990–1992) from Las Vegas (Fax transmission, R.L. Morris, University of Nevada, Reno, Cooperative Extension, to S. LeStrange; July 28, 1997; ACC: MOL.19990629.0319). High and low estimates were considered for Las Vegas.

The Jensen-Haise equation resulted in values that were about 1 inch lower than the modified-Penman estimates during November–January, but as much as 4 inches higher during June–August (Figure A-1). Annual reference ET calculated for the proposed location of the critical group (92.7 inches, Table 3) was higher than that calculated for Pahrump (84.8 inches) and near the high end of the range of values calculated for Las Vegas (84.1–96.7 inches). It is expected that ET for the proposed location of the critical group would be slightly lower than the maximum for Las Vegas because the weather data used to calculate ET at that site (838 m; CRWMS M&O 1999c, Table 1-1 on p. 6) came from a site about 180 m higher than the elevation in Las Vegas (659 m; Devitt et al. 1995a, Table 1 on p. 68). The monthly ET values calculated for the proposed location of the critical group using the Jensen-Haise equation also are within the range or higher than those reported for other locations in the southwestern U.S. (Devitt et al. 1992, Table 2 on p. 719; UCCE 1987, Figure 1 on p. 3; Devitt et al. 1995a, Figure 3 on p. 77). Therefore, the results of the Jensen-Haise equation used in this analysis are valid, conservative estimates of monthly reference ET.

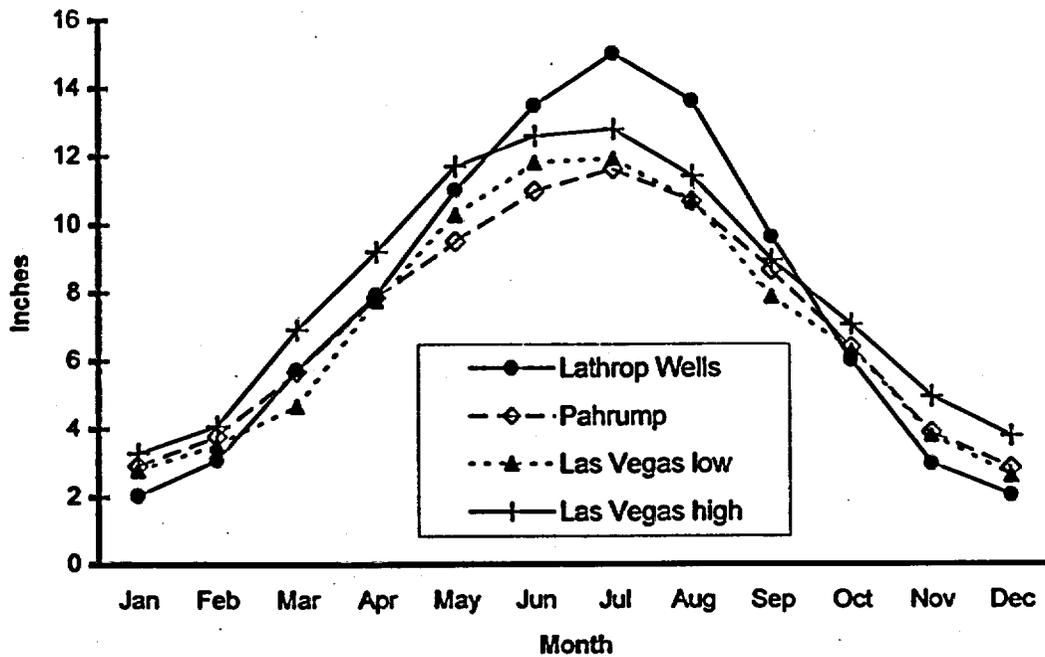


Figure A-1. Reference evapotranspiration (in inches) estimated at the proposed location of the critical group (labeled as "Lathrop Wells" in this figure) and measured in Pahrump (Contact Report; S.L. LeStrange to G.D. McCurdy, Western Regional Climate Center, Reno Nevada; including computer code, weather data, and results of equation. ACC: MOL.19990323.0175) and Las Vegas. (Fax transmission, R.L. Morris, University of Nevada, Reno, Cooperative Extension, to S. LeStrange; July 28, 1997; ACC: MOL.19990629.0319).

APPENDIX B
CONFIRMATION OF A DEEP PERCOLATION VALUE

APPENDIX B. CONFIRMATION OF A DEEP PERCOLATION VALUE

Two equations were used to confirm the validity of a default deep percolation value of 6 inches. These equations use the same data on salt tolerance of crops, but use different methods to determine the leaching requirement (LR), which is the minimum fraction of the total applied water that must pass through the root zone to prevent a reduction in crop yield due to salt accumulation. These calculations were done only for tall fescue, which is less salt tolerant than bermudagrass (Martin et al. 1991a, Table 10-10 on p. 223), and therefore requires a higher level of percolation.

Equation 1. Martin et al. (1991a, pp. 224 through 226) present a method for approximating LR and using an iterative calculation to determine the total annual irrigation depth required to maintain an appropriate salt balance. Iteration is required because one of the inputs, irrigation depth, is not known. Known values for this equation are:

ET_c = evapotranspiration for tall fescue = 85 inches (Table 3)

P = Precipitation = 3.6 inches (CRWMS M&O 1999a, parameter 553).

EC_i = Electrical conductivity of irrigation water = 0.51 dS/m. Calculated as the average conductivity of water from 31 irrigation or domestic wells (Table B-1) located in the village of Amargosa Valley (formerly Lathrop Wells) or west of State Route 373 and south of Highway 95 in Amargosa Valley (McKinley et al. 1991, pp. 9 through 17). These data are skewed somewhat toward low values; only 9 of the 31 measurements are above the mean. These nine wells are at least 9 km from the intersection of State Route 373 and U.S. Highway 95 and the eight most saline wells are more than 16 km south or southwest of that intersection. These most saline wells are located near the Nevada-California border where the water table is much shallower. Thus, the mean of 0.51 dS/m is a reasonable conservative (i.e., high) estimate of salinity expected within the region being evaluated for the reference group.

EC_t = electrical conductivity at salt tolerance threshold = 3.9 dS/m (Martin et al. 1991a, Table 10-10 on p. 223). This is the salinity of irrigation water at which the productivity of tall fescue begins to be affected.

Determination of deep percolation requires the following steps:

1. Calculate the ratio of the electrical conductivity at the salt tolerance threshold to the electrical conductivity of irrigation water: $EC_t:EC_i = 3.9 \text{ dS/m} \div 0.51 \text{ dS/m} = 7.65$
2. Determine the LR using Figure 10-13 of Martin et al. (1991a, p. 225) ≈ 0.05 (Figure 10-13 shows L_r reaching a lower asymptote of about 0.05 at ratios greater than about 3.5).
3. Calculate annual depth (in inches) of irrigation water (I_i) required to prevent a decrease in production:

$$I_i = \frac{ET_c}{1 - L_r} - P = \frac{85}{1 - 0.05} - 3.6 = 85.9,$$

4. Calculate the electrical conductivity of applied water (EC_w) (i.e., diluted by rainfall):

$$EC_w = \frac{EC_i I_i}{I_i + R_i} = \frac{0.51(85.9)}{85.9 + 3.6} = 0.49.$$

5. Determine a new LR based on the ratio of electrical conductivity at the salt tolerance threshold to the electrical conductivity of applied water: $EC_t:EC_w$ ($3.9/0.49 = 7.96$). From Figure 10-13 of McKinley et al. (1991), $LR \approx 0.05$.
6. If necessary, recalculate I_i based on the new LR. Because LR does not change at such high ratios, this step and additional iteration is not necessary. Annual depth of irrigation water required to prevent a decrease in production is 85.9 inches.

Thus, the amount of water required for deep percolation in addition to the 85 inches needed for evapotranspiration is 0.9 inches ($85.9 - ET_c$).

Equation 2. Donahue et al. (1997, pp. 271 through 273) present an equation for LR that is based on the amount of water needed for leaching salts that is in addition to that needed to wet the root zone. For this equation to be used with the data available, one must assume that irrigation is sufficiently applied so that the entire root zone is wetted. Although this assumption may not always be met, completely wetting the root zone is the most efficient method for irrigating; thus, it is valid to assume that this assumption usually will be met.

This equation requires two inputs.

EC_i = Electrical conductivity of irrigation water = 0.51 dS/m (Table B-1).

EC_{dw} = Electrical conductivity causing a 50 percent decrease in yield = 13.33 dS/m. Calculated as yield reduction threshold + (50/yield reduction per unit of salinity increase) = 3.9 dS/m + (50 + 5.3 dS/m) = 13.3 dS/m. Yield reduction values for tall fescue are from Table 10-10 of Martin et al. (1991a, p. 223).

LR is calculated as:

$$LR = \frac{EC_i}{EC_{dw}} = \frac{0.51 \text{ dS/m}}{13.33 \text{ dS/m}} = 0.038$$

This value is similar to that approximated above using Martin et al (1991a, Figure 10-10).

The LR is then multiplied by the total amount of water applied via irrigation (0.038×85 inches) to obtain a deep percolation value of 3.3 inches.

This value is slightly higher than that obtained above using the equation of Martin et al. (1991a, pp. 224 through 226) because Martin et al. (1991a, pp. 224 through 226) account for the addition of salt-free precipitation (in step 3). However, both values are substantially below the default value of 6 inches. Thus, 6 inches is a valid assumption for this analysis.

Table B-1. Electrical conductivity of 31 wells in Amargosa Valley located in the village of Amargosa Valley (formerly Lathrop Wells) or south and west of the intersection of U.S. Highway 95 and State Route 373 (McKinley et al. 1991, pp. 9 through 17).

Site Number	Distance (km) ^a	Electrical Conductivity (dS/m) ^b
37	0.09	0.49
34	3.59	0.34
35	4.33	0.33
36	4.87	0.34
63	9.01	0.65
57	9.13	0.30
60	9.73	0.43
58	9.79	0.31
61	9.84	0.37
59	10.18	0.32
65	12.95	0.30
66	13.36	0.31
53	13.86	0.32
54	15.10	0.33
44	15.44	0.34
43	15.96	0.37
51	16.04	0.35
55	16.33	0.34
77	16.77	0.80
76	17.17	0.38
73	17.87	0.31
56	18.03	0.83
47	18.54	1.07
75	18.73	0.29
42	18.74	0.95
78	18.88	0.28
74	18.90	0.35
39	20.04	0.98
72	20.27	1.29
40	20.71	0.96
89	25.60	0.70
Average		0.51

^a Distance from the intersection of U.S. Highway 95 and State Route 373 to the well.

^b Converted from $\mu\text{S/cm}$ (units used by McKinley et al. 1991, pp. 14 through 17) to dS/m using the equation $\text{dS/m} = 0.001(\mu\text{S/cm})$.

ATTACHMENT A

DOCUMENT INPUT REFERENCE SHEETS

**OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
DOCUMENT INPUT REFERENCE SHEET**

1. Document Identifier No./Rev.:		Change:	Title:						
ANL-MGR-MD-000001, REV 0		0	Input Parameter Values for External and Inhalation Radiation Exposure Analysis						
Input Document		3. Section	4. Input Status	5. Section Used In	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version							Unqual.	From Uncontrolled Source	Un-confirmed
2a	CRWMS M&O 1999a. Climatological Tables from 1988-1997 Meteorological Data From Site 1 through Site 9 EFPD Meteorological Sites. Las Vegas, Nevada: CRWMS M&O. DTN: MO9903CLIMATOL.001. INITIAL USE	Parameters: 553, 594, and 595	TBV-3000	4.1.5#1, #2, & #3; 7; Appendix A and B	Average monthly precipitation, (parameter 553), solar radiation (594) and temperature (595). Verify Q status of these 3 parameters.	1			X
1.									
2.	CRWMS M&O 1999b. Particulate Matter Values from 1989-1997. Las Vegas, Nevada: CRWMS M&O. DTNs: MO98PSDALOG111.000, TM0000000000001.039, TM0000000000001.041, TM0000000000001.042, TM0000000000001.043, TM0000000000001.079, TM0000000000001.082, TM0000000000001.084, TM0000000000001.096, TM0000000000001.097, TM0000000000001.098, TM0000000000001.099, TM0000000000001.105, TM0000000000001.108. INITIAL USE	Parameter 1078	TBV-3198	4.1.1, 6.1, 7	Inhalable particulate matter. Parameter needs to be qualified.	1	X		
3.	Buck, A 1981. "New Equations for Computing Vapor Pressure and Enhancement Factor," <i>Journal of Applied Meteorology</i> , 20, 1527-1532. Boston, Massachusetts: American Meteorological Society. TIC: 239065.	p. 1532	N/A	Appendix A	Equation used to calculate saturated vapor pressure at a given temperature.	N/A	N/A		
4.	CRWMS M&O 1997. <i>Meteorological Monitoring Report, Particulate Matter Ambient Air Quality Monitoring Report January through December 1996</i> . BA0000000-01717-5705-00001 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980416.0733	p. 4	N/A	4.1.1	Description of methods for collecting PM-10 data	N/A	N/A		

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2. Technical Product Input Source Title and Identifier(s) with Version							Unqual.	From Uncontrolled Source	Un-confirmed
5.	CRWMS M&O 1999c. <i>Environmental Baseline File: Meteorology and Air Quality</i> . B00000000-01717-5705-00126. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990302.0186	Tables 1-1, 2-3, and A-9; Fig. 1-1	N/A	4.1.1; 4.1.5 #1, #2, & #3; Appendix A	Descriptive summary of climate data used in analysis.	N/A	N/A		
6.	CRWMS M&O 1999d. <i>Identification of the Critical Group (Consumption of Locally Produced Food and Tap Water)</i> . ANL-MGR-MD-000005 REV 00A. Las Vegas, Nevada: CRWMS M&O. ACC: TBD INITIAL USE	pp. 22-23	TBV-3199	Sections 1, 4, 4.2, 5.2 #3, 6.3, 6.5, 7	Characteristics of population in Amargosa Valley, Report needs to be completed and placed in a controlled source.	1	X		
7.	CRWMS M&O 1999e. <i>Meteorological Monitoring Program 1997 Summary Report</i> . B00000000-01717-5705-00107 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990804.0287.	Figure 3-5	N/A	4.1.1	Description of the location where particulate matter data were collected.	N/A	N/A		
8.	CRWMS M&O 1999f. <i>Development Plan for Input Parameter Values for External and Inhalation Radiation Exposure Analysis</i> . TDP-MGR-MD-000001. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990714.0233.	Entire	N/A	1	Development Plan for Analysis and Model Report; reference only.	N/A	N/A		
9.	CRWMS M&O 1999g. <i>Activity Evaluation: Scientific Investigation of Radiological Doses in Biosphere</i> . B00000000-01717-2200-00169. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990222.0091.	Entire	N/A	2	Activity Evaluation for Analysis and Model Report; reference only.	N/A	N/A		
10.	Devitt, D.A.; Morris, R.L.; and Bowman, D.C. 1992. <i>Evapotranspiration, Crop Coefficients, and Leaching Fractions of Irrigated Desert Turfgrass Systems</i> . <i>Agronomy Journal</i> , 84, 717-723. Madison, Wisconsin: American Society of Agronomy, Inc. TIC: 244&77. INITIAL USE	Table 3, pp. 717-723	TBV-3200	Sections 4, 4.1.5 #4, 5.5 #1, 6.5, Table 4, Appendix A	Crop coefficient for bermudagrass. Source of data needs to be classified as accepted.	1	X		

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2. Technical Product Input Source Title and Identifier(s) with Version							Unqual.	From Uncontrolled Source	Un-confirmed
11.	Devitt, D.A.; Kopec, D.; Robey, M.J.; Morris, R.L.; Brown, P.; Gibeault, V.A.; and Bowman, D.C. 1995a. Climatic Assessment of the Arid Southwestern United States for Use in Predicting Evapotranspiration of Turfgrass. <i>Journal of Turfgrass Management</i> , 1, 75-81. Binghamton, New York: Haworth Press, Inc. TIC: 245203	pp. 75-81	N/A	4.1.5 #4, Appendix A	Influence of climate on evapotranspiration (ET). Used to corroborate ET calculation.	1	N/A	N/A	
12.	Devitt, D.A.; Neuman, D.S.; Bowman, D.C.; and Morris, R.L. 1995b. Comparative Water Use of Turfgrasses and Ornamental Trees in an Arid Environment. <i>Journal of Turfgrass Management</i> , 1, 47-63. Binghamton, New York: Haworth Press, Inc. TIC: 244814. INITIAL USE	Figure 2, pp. 47-63	TBV-3201	Sections 4, 4.1.5 #4, 6.5, Table 4	Crop coefficient for tall fescue. Source of data needs to be classified as accepted.	1	1		
13.	DOE (U.S. Department of Energy) 1998. Quality Assurance Requirements and Description for the Civilian Radioactive Waste Management Program. DOE/RW-0333P REV. 8. Washington, D.C. U.S. Department of Energy. ACC: MOL19980601.0022.	Entire	N/A	2, 4.1.5	Quality Assurance Requirements and Description program followed; reference only	N/A	N/A		
14.	Donahue, R.L.; Miller, R.W.; and Shickluna, J.C. 1977. <i>Soils: An Introduction to Soils and Plant Growth</i> . Fourth Edition. Englewood Cliffs, NJ: Prentice Hall, Inc. TIC: 242506.	pp. 271-273	N/A	Appendix B	Equation used to corroborate assumption for deep percolation value.	N/A	N/A		
15.	Dyer, J.R. 1999. "Interim Guidance Pending Issuance of New U.S. Nuclear Regulatory Commission (NRC) Regulations for Yucca Mountain." Letter from J.R. Dyer (DOE/YMSCO) to D.R. Wilkins (CRWMS M&O), OL&RC:AVG:1435, June 18, 1999, with enclosure. ACC: MOL19990623.0026; MOL.19990623.0027.	p. 19 of enclosure	N/A	1, 4, 4.1.1, 4.1.5, 4.2, 5.2 #3, 6.3, 6.6	DOE guidance on using proposed NRC rules defining the critical group.	N/A	N/A		

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2. Technical Product Input Source Title and Identifier(s) with Version							Unqual.	From Uncontrolled Source	Un-confirmed
16.	EPA (Environmental Protection Agency) 1994a. <i>Quality Assurance Handbook for Air Pollution Measurement Systems, Volume II: Ambient Air Specific Methods (Interim Edition)</i> . EPA/600/R-94/038b. Research Triangle Park, NC: Office of Research and Development. TIC: 242101.	Section 2.11	N/A	4.1.1	Description of methods used to measure PM ₁₀ .	N/A	N/A		
17.	EPA 1994b. <i>Methods for Derivation of Inhalation Reference Concentrations and Application of Inhalation Dosimetry</i> . EPA/600/8-90/066F. Research Triangle Park, NC: Office of Research and Development. TIC: 245087.	Figure 3-3	N/A	4.1.1	Confirmation of selection of PM ₁₀ data as mass loading input.	N/A	N/A		
18.	EPA 1997a. <i>Exposure Factors Handbook. Volume I. General Factors</i> . EPA/600/P-95/002Fa. Washington, D.C.: Office of Research and Development. TIC: 241060.	pp. 5-1 through 5-27	N/A	6.3	Review of chronic breathing rate values.	N/A	N/A		
19.	EPA 1997b. <i>Exposure Factors Handbook. Volume III. General Factors</i> . EPA/600/P-95/002Fc. Washington, D.C.: Office of Research and Development. TIC: 241062	Table 15-7 and Table 15-20	N/A	5.2	Description of time spent outdoors	N/A	N/A		
20.	ICRP (International Commission on Radiological Protection) 1975. <i>Report of the Task Group on Reference Man</i> . ICRP Pub. No. 23. Tarrytown, New York: Pergamon Press. TIC: 237218.	pp. 346-347, and entire	N/A	6.3	Review of chronic breathing rate values.	N/A	N/A		
21.	LaPlante, P.A.; and Poor, K. 1997. <i>Information and Analyses to Support Selection of Critical Groups and Reference Biospheres for Yucca Mountain Exposure Scenarios</i> . CNWRA-97-009. San Antonio, Texas: Center of Nuclear Waste Regulatory Analyses. TIC: 236454.	p. 2-23	N/A	6.2	Review of time spent outdoors by an agricultural worker.	N/A	N/A		
22.	Las Vegas Valley Water District Undated. <i>The All Seeing All Knowing Desert Lawn Care Manual</i> . Las Vegas, Nevada: Las Vegas Valley Water District. TIC: 244376	pp. 10-13	N/A	6.5, 6.6	Corroboration of irrigation rates for turfgrass.	N/A	N/A		

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1. Document Identifier No./Rev.:		Change:	Title:						
ANL-MGR-MD-000001, REV 0		0	Input Parameter Values for External and Inhalation Radiation Exposure Analysis						
Input Document		3. Section	4. Input Status	5. Section Used In	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version							Unqual.	From Uncontrolled Source	Un-confirmed
23.	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, UC-721. Albuquerque, New Mexico: Sandia National Laboratories. TIC: 231133.	Entire	N/A	1.6.1, 6.2, 6.4, Table 4	GENII-S computer code for which input parameters are required.	N/A	N/A		
24.	Martin D.L.; Gilley, J.R.; and Skaggs, R.W. 1991a. "Soil Water Balance and Management." <i>Managing Nitrogen for Groundwater Quality and Farm Profitability</i> , 198-255. Madison, Wisconsin: Soil Science Society of America. TIC: 243453.	pp. 200-204 and 223-226	N/A	4.1.5.#4, 5.5 #1, 6.5, Table 4, Appendix B	Description of how to calculate evapotranspiration and calculation used to corroborate deep percolation value.	N/A	N/A		
25.	Martin D.L.; Gilley, J.R.; and Skaggs, R.W. 1991b. "Evapotranspiration Equations" <i>Managing Nitrogen for Groundwater Quality and Farm Profitability</i> , 333-338. Madison, Wisconsin: Soil Science Society of America. TIC: 238376.	pp. 334-336	N/A	6.5, Appendix A and B	Equation used to calculate evapotranspiration.	N/A	N/A		
26.	McKinley, P.W.; Long, M.P; and Benson, L.V. 1991. <i>Chemical Analyses of Water from Selected Wells and Springs in the Yucca Mountain Area, Nevada and Southeastern California</i> . Open-File Report 90-355. Denver, Colorado: U.S. Geological Survey. TIC: 201912.	pp. 9-17	N/A	Appendix B	Salinity of groundwater in Amargosa Valley. Used to corroborate assumed value of deep percolation.	N/A	N/A		
27.	Morris, B.; and Johnson, W. 1986. <i>Grass Selection for the Urban Mojave Desert Landscape</i> . Fact Sheet 86-72. Reno, Nevada: University of Nevada, Cooperative Extension. TIC: 244377.	pp. 1-4	N/A	6.5	Types of turfgrass commonly grown in southern Nevada. Used to corroborate distribution of home irrigation rate.	N/A	N/A		
28.	Morris, B.; and Johnson, W. 1991. <i>Maintaining Hybrid Bermudagrass for Urban Mojave Desert Landscapes</i> . Fact Sheet 91-24. Reno, Nevada: University of Nevada, Cooperative Extension. TIC: 244378.	pp. 1-4	N/A	6.5, 6.6	Irrigation requirements of bermudagrass, used to corroborate calculated value.	N/A	N/A		

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2. Technical Product Input Source Title and Identifier(s) with Version							Unqual.	From Uncontrolled Source	Un-confirmed
29.	Morris, B.; and Van Dam, J. 1989. <i>Maintaining Tall Fescue Turfgrass in Urban Mojave Desert Landscapes</i> . Fact Sheet 89-25. Reno, Nevada: University of Nevada, Cooperative Extension. TIC: 244506.	pp. 3-4	N/A	6.6	Irrigation requirements of tall fescue. Used to corroborate calculated value.	N/A	N/A		
30.	Napier, B.A.; Peloquin, R.A.; Strenge, D.L.; and Ramsdell, J.V. 1988. <i>GENII - The Hanford Environmental Radiation Dosimetry Software System, Volume 1: Conceptual Representation</i> , PNL-6584-Vol.1. Richland, Washington, Pacific Northwest Laboratory. TIC: 206898.	p. 4.58	N/A	5.5. #1	Inferred value of deep percolation in GENII-S code.	N/A	N/A		
31.	NRC (Nuclear Regulatory Commission) 1977. <i>Calculations of Annual Doses to Man From Routine Releases of Reactor Effluents for the Purpose of Evaluating Compliance With 10 CFR Part 50, Appendix I</i> . NRC Regulatory Guide 1.109. Washington, D.C.: Office of Standards Development. TIC: 222641	p. 1.109-43	N/A	5.2 #1, 6.2	Basis of assumption for indoor shielding factor.	N/A	N/A		
32.	NRC 1995. <i>NRC Iterative Performance Assessment Phase 2: Development of Capabilities for Review of a Performance Assessment for a High-Level Waste Repository</i> . NUREG-1464. Washington, D.C.: Nuclear Regulatory Commission. TIC: 221527.	p. 7-10	N/A	6.2	Statement about percent of time a person spends outdoors; used to corroborate values developed in analysis.	N/A	N/A		
33.	UCCE (University of California Cooperative Extension) 1987. <i>Using Reference Evapotranspiration (ET_r) and Crop Coefficients to Estimate Crop Evapotranspiration (ET_c) for Agronomic Crops, Grasses, and Vegetable Crops</i> . Leaflet 21427. Berkeley, California: University of California Cooperative Extension, Division of Agriculture and Natural Resources. TIC: 243488.	pp. 1-12	N/A	4.1.5 #4, 6.5, Appendix A	Examples of how to calculate evapotranspiration and use crop coefficients; used to defend and explain methods used in analysis.	N/A	N/A		
34.	Contact Report; S.L. LeStrange to G.D. McCurdy, Western Regional Climate Center, Reno Nevada; including computer code, weather data, and results of equation. MOL.19990323.0175.	entire	N/A	Appendix A	Evapotranspiration in Pahrump; used to corroborate calculation of evapotranspiration used in analysis.	N/A	N/A		

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35.	Fax transmission, R.L. Morris, University of Nevada, Reno, Cooperative Extension, to S. LeStrange; July 28, 1997; ACC: MOL 19990629.0319	page 3	N/A	Appendix A	Evapotranspiration in Las Vegas, used to corroborate the calculation of evapotranspiration used in analysis.	N/A	N/A		
36.	40 CFR 50, Appendix J (1996). Reference Method for the Determination of Particulate Matter as PM10 in the Atmosphere.	p. 65-70	N/A	4.1.1	Descriptive information on methods used to measure particulate matter.	N/A	N/A		
37.	40 CFR 50.6 1996. Primary and Secondary Ambient Air Quality Standards for PM10.	p. 7	N/A	4.1.1	EPA National Ambient Air Quality Standards for particulate matter. Used to corroborate validity of PM ₁₀ data used.	N/A	N/A		
38.	64 FR 8640-8678 (1999). Disposal of High-Level Radioactive Wastes in a Proposed Geologic Repository at Yucca Mountain, Nevada.	pp. 8640-8678	N/A	1.4.2, 6.3, 7	Characteristics of the critical group proposed by the NRC. Used to explain basis of characteristics used.	N/A	N/A		

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Interoffice Correspondence
Civilian Radioactive Waste Management System
Management & Operating Contractor



TRW Environmental
Safety Systems Inc.

QA:QA

Subject:
Assessment of Heat Loss Through the
Drift Scale Test Bulkhead

Date:
October 21, 1999
LV.NEPO.TEST.RAW.10/99-373

From:
R. A. Wagner
Ralph Wagner

To:
M. T. Peters

cc:
See Below

Location/Phone:
SUM1/820B
702-295-5623

BACKGROUND

Over the past several months, the issue of heat loss through the Drift Scale Test (DST) bulkhead has been discussed and analyzed. Much of this discussion has been documented in three informal reports entitled "Thermal Test Progress Report No. 1, 2, and 3" (see Enclosure Nos. 1, 2, and 3). The issue of heat loss was initially addressed during the design of the bulkhead in which it was not considered necessary for the heated drift to be sealed air tight (DST Design and Forecast Results report; BAB000000-01717-4600-00007; published December 11, 1997). Rather, the bulkhead was to be protective and to serve as a primary thermal barrier to retard conductive heat loss. This type of bulkhead would allow workers and visitors close access to the DST with minimal risk. In addition to internal discussions among the thermal test team, the NRC requested a U.S. Department of Energy/Nuclear Regulatory Commission (DOE)/(NRC) Appendix 7 meeting to further discuss this topic. This meeting was held April 28, 1999 in Las Vegas. A summation of the meeting was circulated by e-mail on June 13, 1999 by Michael Scott (see Enclosure No. 4). Key issues related to bulkhead heat loss raised by the NRC are as follows: continuously monitoring vapor and air escaping the bulkhead; evaluating the efficacy of redundant calibrated manometers; and evaluating existing ventilation data in assessing heat loss.

SUMMARY/RESULTS

In summary, the original plan/design of the DST bulkhead is still considered satisfactory. The bulkhead was simply intended to provide a protective and primary thermal barrier to allow personnel, both visitors and workers, to observe the heated drift and to work in close proximity to the bulkhead/heated drift with minimal risk. After much additional scrutiny, extensive and more accurate characterization of the heat loss through the bulkhead is considered difficult, problematic, and unnecessary.

Heat loss is attributed to a combination of the three primary modes of heat transfer: conductive, convective, and radiative. Determination of the total heat loss or individual modes of heat transfer is nontrivial for several reasons including:

- Convective Heat Loss
 - irregular shape of the bulkhead (regardless, conductive heat loss is considered small compared to convective heat loss).

- Convective Heat Loss
 - the inherent leakage through the bundles of power-cables and instrument-wiring pathways through the bulkhead,
 - substantial ventilation on the cool side of the bulkhead greatly impedes the ability to measure heat loss from the bulkhead,
 - the inability to measure low airflow rates should the existing ventilation be greatly reduced,
 - existing ventilation data is not useful for determining heat loss because large volumetric flowrates and limitations of temperature and relative humidity measuring devices, and
 - because of problems cited above, continuous measurement would not be beneficial.
- Radiative Heat Loss
 - with the exception of a minor amount of radiation through the glass windows, radiative heat losses is primarily from the outer surface of the bulkhead. Given this condition, it is a subset of conductive heat loss and can be considered both difficult to measure and a minor component of the overall heat loss.

Ultimately, the need to measure heat loss through the bulkhead hinges on the accuracy of numerically simulating the thermal behavior in the DST. Analyses indicate that an assumed convective boundary condition results in good comparative agreement between measured and simulated temperatures. Thus, the lack of accurate measurements of heat loss can be offset by proper numerical modeling. This approach is preferable to attempting to directly measure heat loss which has proven to be difficult.

DISCUSSION

The following discussion on heat loss through the bulkhead is divided into the three modes of heat transfer losses and an evaluation of a numerical approach to this problem.

Conductive Heat Loss

Much discussion on addressing conductive heat loss through the bulkhead has been documented in three informal progress reports (see Enclosures Nos. 1, 2, and 3). The following is a summary of the approaches and results presented in these informal reports.

Conductive heat loss through the bulkhead initially appeared to be a significant contributor to the total heat loss. Also, it appeared a remedy, insulating the cool side, could be easily and effectively installed. Before insulating, attempts were made to quantify the conductive heat loss by direct measurements. Subsequently, heat flux through seven steel and glass locations was measured with heat flux meters. The total conductive heat loss, based on these measurements, was estimated to be approximately 6 kW. The irregular shape of the bulkhead, especially numerous "fins" or steel-mesh guards that protect the glass windows, make it difficult to accurately extrapolate these conductive heat flux measurements into a single value. Because of the inherent uncertainty to these measurements, the estimate that conductive heat loss is much less than convective heat losses, and newly perceived problems with the installation of insulation; further evaluation of heat loss was focused on convective heat loss.

Radiative Heat Loss

Heat loss through the bulkhead by radiation was not considered because it cannot be measured without good measurement of temperature along the outer side of the bulkhead. As discussed above, the irregular configuration of steel, windows, and cable/wire bundles makes this a formidable and difficult task. Most radiative heat loss is a component of conductive heat loss since the conductive heat loss is dependent on temperature difference across the thickness of the bulkhead materials (e.g. steel plates or glass windows); whereas, radiative heat loss is dependent on the temperature difference between the bulkhead's outer surface and the air. A secondary amount of radiative heat loss is transmitted through the bulkhead's glass windows which comprise a small fraction of the bulkhead's surface area. In summary, most of the radiative heat loss is a subset of the conductive heat loss and therefore is not considered significant.

Convective Heat Loss

As discussed in Enclosures Nos. 1, 2, and 3, measurement of convective heat loss is difficult for several reasons. The leakage through the three sets of power cables and single set of instrument wiring is essentially unstoppable. Other leaks exist around the periphery and through door and window openings. Attempts to pack and seal the bundles and other leaks have only mitigated, not eliminated, this uncertainty. Another factor is the temporal moisture fluctuations from "barometric pumping" and the dynamics of moisture drying and mobilization in the heated drift and test block. These temporal fluctuations, which are both diurnal and seasonal, are difficult to eliminate because continuous measurements of convective heat loss are not practical.

Whether the convective heat loss is measured from either a liquid-water condensation/collection system or a water-vapor relative humidity detection system, inherent uncertainties will be substantial. Other concepts for measuring convective heat loss through the bulkhead are considered even less applicable. The primary problem with the liquid-water condensation/collection system is (1) the collected sample does not represent the total amount of water vapor loss and (2) the inability to accurately estimate the total amount of water vapor loss. Also, continuous measurements, which would be expensive and cumbersome, would be needed to avoid uncertainties from temporal fluctuations.

The primary problem with the water-vapor relative humidity detection system is the need to reduce the flow of ventilated air on the cool side of the bulkhead to ensure an accurate determination of the amount of water vapor escaping through the bulkhead. The need to significantly reduce the ventilation rate becomes apparent when the rate of moisture loss from the numerically estimated 22 kW convective heat loss (equates to 35 liters of water vapor per hour which requires 1.5 million liters of air per hour to keep the air saturated) is compared to the range of ventilation flow rates between 50 and 150 million liters per hour. This comparison indicates the ventilation rate is 35 to 100 times too large to allow estimation of moisture loss through the bulkhead by measuring relative humidity changes. [Note: Thermal-hydrological analyses by LBNL indicate convective heat loss through the bulkhead is approximately 22 kW].

Complications also exist with accurate measurement of a much slower ventilation flow rate needed to detect the moisture losses through the bulkhead. Based on input from an M&O ventilation analyst, Romeo Jurani, devices available to detect low velocities are listed below

along with respective minimum velocities needed for measurement:

- Anemometers (0.15 m/s)
- Hot-wire anemometers (0.07 m/s)
- Manometer (0.50 m/s)
- Smoke tester (0.05 m/s)...Note: requires diameter of air pathway to be less than 0.5 m

All of these minimum velocities are higher than the maximum velocity (0.02 m/s) needed to detect moisture losses in the 5-m-diameter drift outside the bulkhead.

Ron Green, CNWRA, requested the thermal test team to investigate flowmeters for low flowrates. Specifically, he found a flowmeter distributed by J&W Scientific capable of measuring 10 ml/min. Upon contacting a technical support member, Jason Ellis, it was explained that J&W Scientific flowmeters were designed for application in a laboratory environment for small diameter tubes. Mr. Ellis explained that the technology in their flowmeters would not be applicable to large-diameter tunnels such as those in the DST. Mr Ellis suggested contacting Omega Engineering for low flowrate flowmeters. Omega Engineering technical support member, Gary Palmer, confirmed that it would be difficult to measure velocities lower than 0.05 m/sec. Furthermore, he said spatial variability in flowrate and direction would make it quite difficult to interpret measurements at these low flowrates. Even if the reduced flow of ventilated air could be measured and resulted in a reasonable estimate in moisture loss, the reduced air flow is not representative of actual conditions. Actual ventilation velocities are estimated to range from 0.70 to 2.1 m/s. But as discussed above, these higher velocities make it essentially impractical to measure slight increases in relative humidity from moisture losses through the bulkhead.

Numerical Simulations

Ultimately, the need to directly measure the heat loss through the bulkhead is related to its impact towards producing accurate numerical simulations. Based on qualitative (see Figures 1 thru 3) and quantitative (see Table 1) comparisons of measured and calculated temperatures, it appears additional accuracy in characterization of the bulkhead will not significantly improve the ability to simulate the thermal response in the DST block. Figures 1 thru 3 show good agreement in both temperature magnitude and trend for six representative locations approximately one meter into the rock along the heated drift. In general, the calculated temperatures are slightly greater than measured temperatures. This could be further reduced by modifying the "perfectly-insulated" boundary condition along the bulkhead to allow some conductive heat loss.

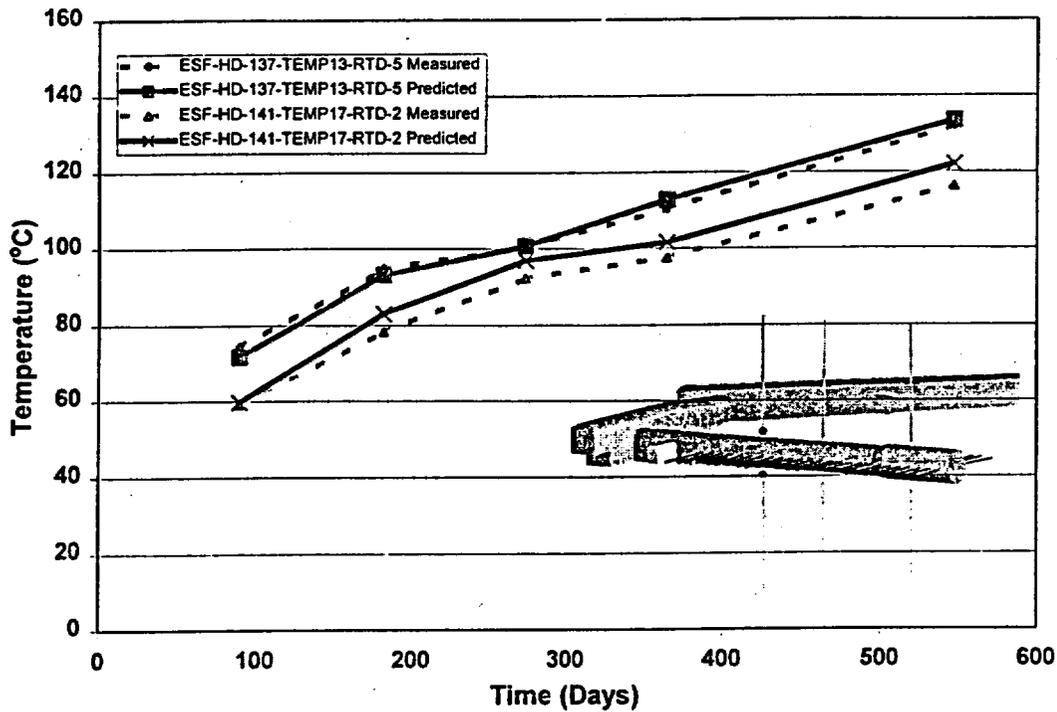


Figure 1. Comparison of Measured and Calculated DST Temperatures approximately 12 meters into the Heated Drift and One Meter into the Roof.

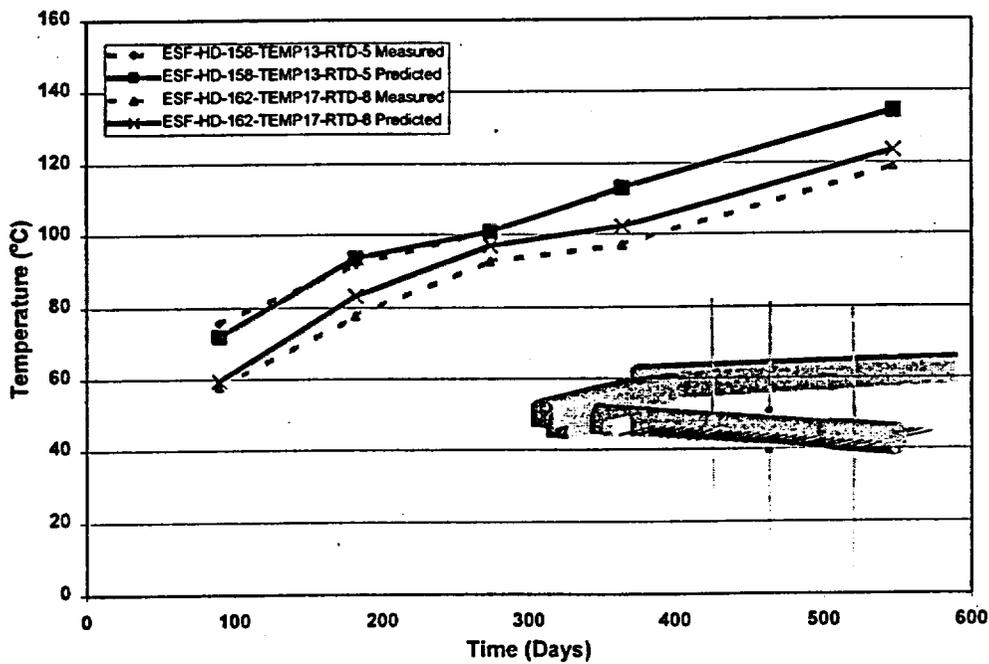


Figure 2. Comparison of Measured and Calculated DST Temperatures approximately 23 Meters into the Heated Drift and One Meter into the Roof.

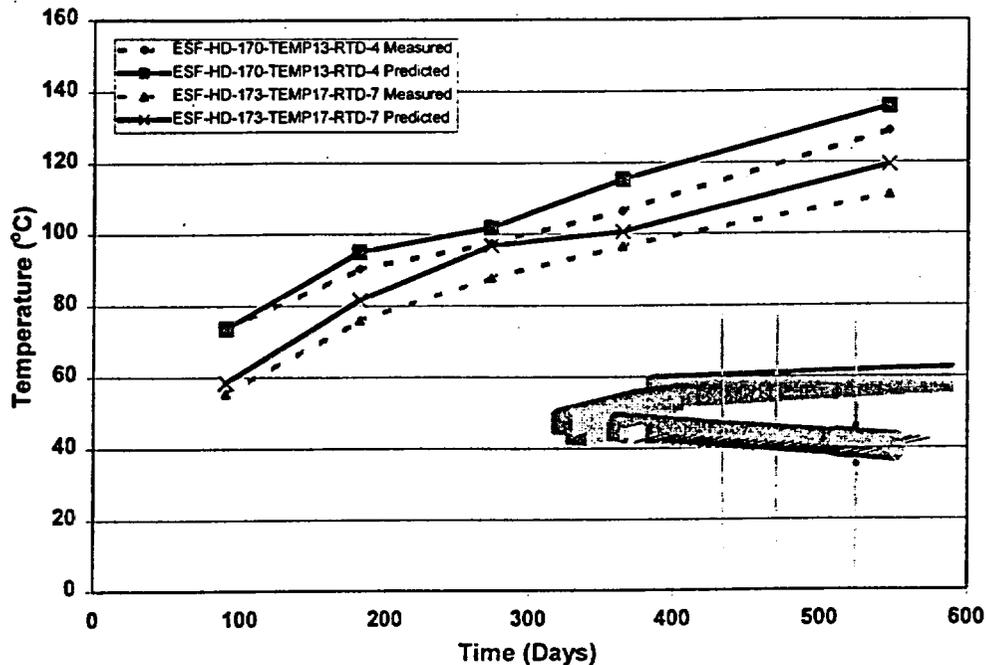


Figure 3. Comparison of Measured and Calculated DST Temperatures Approximately 39 Meters into the Heated Drift and One Meter into the Roof.

Statistical measures, such as weighted root mean square error (WRMSE) and mean error (ME), shown in Table 1 indicate good overall agreement between measured and calculated temperatures throughout the DST block. Approximately 1500 thermal measurements from 23 boreholes were used in this statistical assessment. The thermal-hydrological calculations are from an effective continuum, three-dimensional model of the DST. The ME ranges from +0.8 to +3.2 °C during the initial 18 months of heating. The WRMSE ranges from 4.3 to 8.7 for the same duration. A positive mean error, which is small in this assessment, indicates a slight overprediction of the measured temperatures.

October 22, 1999

Page 7

Table 1. Statistical Measures of Agreement Between Measured and Calculated Temperatures for Effective Continuum Model

Criteria	Time (months)					
	3	6	9	12	15	18
Mean Error (°C)	0.9	1.1	1.6	2.1	2.7	3.4
Weighted Root Mean Square Error (°C)	4.3	5.9	7.0	7.8	8.6	8.7

Note: Mean Error from simulated and measured temperatures of 23 boreholes (133, 137-144, 159-163, 165, 168-175) in the Drift Scale Test.

Since past numerical simulations and corresponding assumptions along with anticipated future refinements to the numerical analyses can account for the heat loss through the bulkhead, direct and difficult measurements of conductive and convective heat loss are not considered necessary.

RAW/dm

Enclosures

1. Moisture Movement Across the Bulkhead
2. Heat Lost Through the DST Bulkhead
3. Conduction and Convection Through the DST Bulkhead
4. DOE/NRC Appendix 7 Meeting on Thermal Testing

cc:

Deborah Barr, USGS, Las Vegas, NV
 S. C. Blair, M&O/LLNL, Livermore, CA
 R. N. Datta, M&O/URSGWCFS, Las Vegas, NV
 A. C. Matthusen, M&O/URSWCFS, Las Vegas, NV
 S. R. Sobolik, M&O/SNL, Albuquerque, NM
 Yvonne Tsang, M&O/LBNL, Berkeley, CA
 D. J. Weaver, M&O/LANL, Las Vegas, NV
 RPC=20 Pages

4.11 Moisture Movement Across the Bulkhead

The Heated Drift is separated from the rest of the thermal testing facility by a bulkhead. The bulkhead is a thermal bulkhead, not a pressure bulkhead. It is made of a steel frame and steel plates and carries the lighting fixtures, viewing windows and the camera door. The bulkhead is insulated on both sides by fiber glass insulation pads.

The relative humidity (RH) inside the Heated Drift dropped to approximately 15 percent during the first 10 days of heating. Thereafter, the RH inside the HD fluctuated between 10 and 25 percent with a peak to peak interval of approximately 4 days. Measured RH in the HD has been inversely tracking the air pressure in the drift. After some forty days of heating, moisture started to flow out of the Heated Drift as evidenced by condensation on various surfaces near the bulkhead and the formation of a puddle on the floor. Such wet conditions near the bulkhead alternated with dry conditions with the latter coinciding with low RH inside the HD.

The Drift Scale Test System, comprised of the HD and the surrounding heated and unheated rock, is not a closed system. The DST block is exchanging moisture and air with its surroundings through the bulkhead and the fractured rock. Outflows coincide with higher RH in the HD and lower barometric pressure.

As the rock immediately surrounding the drift is heated to above the boiling temperature, the pore water in the rock is mobilized and driven outward creating a dry-out zone around the drift. As the mobilized water in the vapor phase moves outward, it condenses when it reaches cooler regions and vaporizes again, as additional thermal pulse reaches it. A boiling zone is thus formed around the dry-out zone. Phase changes occur continuously in the boiling zone causing pressure to build up. When the barometric pressure and the pressure inside the HD are high, steam and water is confined to the boiling zone. When the barometric pressure and the pressure in the HD drop, steam and water escape from the boiling zone moving into the HD via the fractures and causing the RH in the drift to rise, much like what happens in pressure cooker or geyser.

Ways of measuring the heat loss through the bulkhead, both by conduction and convection, have been investigated. A pair of sensitive heat flux meters has been acquired and will be used to measure the heat loss by conduction in the first part of January 1999.

Measuring the loss by convection is difficult and complicated because flow takes place at numerous locations, at various rates and at different temperatures.

4.11 Heat Loss Through the DST Bulkhead

Heat loss through the DST bulkhead was investigated to obtain a better thermal boundary condition for numerical simulations of the DST. In some cases, the thermal boundary condition for the bulkhead was assumed to be perfectly insulated which translate into no heat flux. Given the understanding of the insulation thickness and condition on the "hot" side of the bulkhead, it became apparent that the heat flux through the bulkhead was significant.

The determination of the total heat flux required consideration of both conductive and convective modes of heat transfer. Radiation through the bulkhead was considered negligible. Conductive heat flux was determined with direct (non-Q) measurements by applying a heat flux meter to the seven locations on the bulkhead (see Figure 4.11-1). Five measurement locations were steel (Nos. 1, 2, 4, 5, and 7) and two measurement locations were glass (Nos. 3 and 6). Figure 4.11-1 shows these seven locations and the corresponding heat fluxes in W/m^2 . Measurements of all seven locations were conducted with and without 4-inch thick insulation covering the heat flux meter. For location No. 1, three thicknesses of insulation were used (2, 4, and 6). By covering the heat flux meter with insulation, the influence of the nearby ventilation exhaust could be assessed.

Results indicate the mean conductive heat loss through the bulkhead is approximately 5 kW. Also, forced convection from the ventilation system increases conductive heat loss by approximately an order of magnitude. The 4-inch thick insulation appeared adequate to ensure the ventilation exhaust did not remove significant heat from the bulkhead.

Convective heat loss was estimated by considering how much water vapor was removed from a small diameter pipe in the bulkhead during a 60-minute sampling period. By considering the condensed water's heat of vaporization, it is possible to calculate the convective heat loss. Results from Table 4.11-1 indicate an approximate 0.5 kW heat loss. The total convective loss is dependent on the total pathways through the bulkhead including leakage along the periphery, doors, and wire/cable bundles. These total estimates indicate the convective heat loss through the bulkhead may vary from 2kW to 20kW. Because quantifying all pathways is difficult, accurate measurement of these type of losses is nontrivial.

Given the anticipated minor impact of these heat losses on the overall performance of the DST, remedies for reduction of heat loss should be straightforward, beneficial, and inexpensive.

Heat loss through the bulkhead accommodates, to some extent, the desire to keep the design thermal loading in the center of the DST block lower than the outer portion. This thermal load design increases the likelihood of observing reflux near and possibly into the heated drift during the cooling phase. Power was intentionally reduced in the floor heaters to 80 percent (54 kW) while maintaining the total power in the outer and inner wing heaters at 86 kW and 57 kW, respectively. Conversely, the heat loss across the bulkhead is nonuniform which would complicate proper modeling. Also, it is prudent, if feasible, to mitigate uncertainties.

Based on the above factors and much discussion among the thermal test team, the following actions were recommended.

- Re-pack the periphery of the bulkhead and other leaks to substantially reduce the amount of water vapor escaping through this pathway.

- Re-direct the ventilation such that it does not blow directly onto the bulkhead.
- If high-temperature spray foam can be located, spray into voids of the wiring and cable bundles to reduce vapor flow.
- Evaluate sensitivity of numerical predictions to the uncertainties associated with bulkhead heat losses.

Table 4.11-1 Convective Heat Loss Through the Bulkhead From Vapor Removal System.

DATE	AIR TEMP IN HEATED DRIFT (°C)	RELATIVE HUMIDITY IN HEATED DRIFT (%)	CONDENSATE RECOVERD (ml/hour)	CONVECTIVE HEAT LOSS (kW)
5 Aug 98	126	8.6	600	0.38
26 Aug 98	135	11.4	870	0.54
31 Aug 98	134	10.8	800	0.50

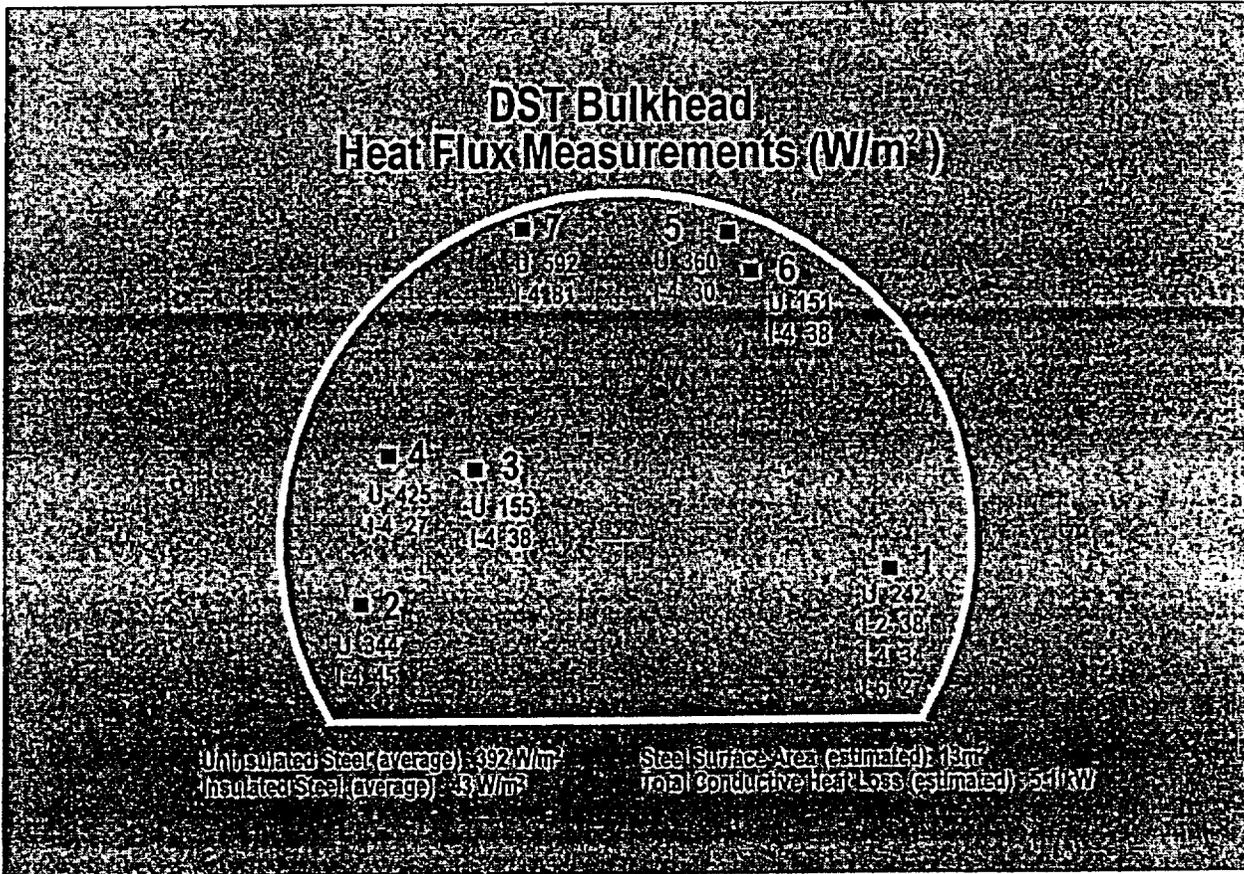


Figure 4.11-1 Heat Flux Measurements on the Bulkhead.

3.11 Conduction and Convection Through the DST Bulkhead

The loss of heat through the DST bulkhead has been an ongoing concern since the planning and design phases of the DST. Heat loss can be divided into conductive and convective fluxes. Conductive heat loss occurs through the bulkhead's steel construction; whereas the convective heat loss is from water vapor escaping through bulkhead leaks such as the power cables, sensor wiring, doorways, and periphery. It appears the measurement of convective heat fluxes is more difficult than the measurement of conductive heat fluxes. The following discussion provides a chronology of activities associated with the bulkhead's heat loss.

Design Considerations

The bulkhead was designed to perform as a thermal barrier but not as a hydrological barrier. Water vapor was not intended to be trapped. Even though the bulkhead was designed to be a thermal barrier, it was never intended to be perfectly insulated. Consequently, some heat loss was anticipated. This condition is considered acceptable because of the ability to numerically simulate the heat flux and limitations of constructing a thermal bulkhead.

Other design aspects of the DST need to be considered when evaluating the impact of heat loss through the bulkhead such as the existence of an open system in the DST block. An open system is known to exist because of the negligible retardation in barometric pressure between measurements in the local rock mass and the north portal pad. The existence of an open system in the fracture network provides implies numerous pathways, in addition to the bulkhead, for water vapor movement. The DST was designed to overdrive heating in order to expedite the test. This fast heating rate results in additional heat loss through the bulkhead. Also, it was anticipated that numerical simulations/modeling of the DST could accommodate uncertainties, such as bulkhead heat loss, through implementation of suitable boundary conditions and proper sensitivity analyses. Furthermore, the DST design anticipated the need for refinements in the test such as those associated with bulkhead heat loss.

Initial Observations

Shortly after the DST heaters were activated, moisture accumulations on the bulkhead's cool side were observed. Investigations of this phenomenon resulted in an understanding that the moisture was largely condensed water vapor that escaped the bulkhead. The observed moisture, estimated to be 100s of liters, has been a small fraction of the estimated 10 million liters of water mobilized in the test block.

Figure 3.11-1 shows graphically another observation stemming from this initial observation which is the inverse relationship of barometric pressure and relative humidity measured in the heated drift. This "barometric pumping" retards the flow of water vapor through the bulkhead, which is a measure of convective heat loss, during high pressure days. Conversely, the flow of water vapor through the bulkhead increases during low pressure days.

These initial observations led to installation of additional thermal and moisture probes along the roof's centerline on the bulkhead's cool side. These instruments facilitate the interpretation of moisture accumulation on the outside of the bulkhead. Also, these initial observations provided insights on repository performance including the potential for natural removal of heat and moisture as well as the likelihood of low relative humidity in the heated drift.

Refinements

Several refinements in the DST have either occurred or are anticipated. Specifically, baffles have been placed over the ventilation outlets near the bulkhead to reduce the amount of forced convection on the bulkhead. Water vapor leaks in the bulkhead, such as those in the camera door and cable outlets, have been sealed to the extent practical. Sealing is intended to mitigate convective heat loss through the bulkhead. A water collection system was developed to estimate convective heat losses through the bulkhead. Currently, improved methods for measuring conductive and convective heat losses through the bulkhead are being evaluated.

Recent Observations

Conductive heat losses have been measured on four occasions as shown in Figure 3.11-2. Results indicate the estimated conductive heat loss through the bulkhead ranges from 5 to 7 kW. Similarly, convective heat losses have been measured from nine different samplings taken from the water collection system. As shown in Table 3.11-1, the convective heat loss through the 1.5 inch-diameter opening in the bulkhead ranges between 0.2 and 0.6 kW. Total convective heat loss is estimated to range from 4 kW to 30 kW. Other observations indicate the presence of a convection cell around the bulkhead and a transient drying trend in the heated drift.

Future Activities

Future activities include ongoing monitoring of the thermal-hydrological behavior in terms of measurements and numerical simulations. This activity includes sensitivity analyses to better determine the impact of heat loss through the bulkhead on the ability to replicate the T-H behavior. Also, existing methods for measuring conductive and convective heat loss through the bulkhead are being re-evaluated to improve accuracy.

Table 3.12-1 Convective Heat Loss from Vapor Removal System.

Date	HD Air Temp (°C)	Relative Humidity (%)	Air Pressure (KPa)	Condensate Removed (ml/hour)	Convective Heat Loss (kW)
07/29/1998	133	15.2	90.0	305	0.19
08/05/1998	126	8.6	90.4	600	0.38
08/26/1998	135	11.4	89.9	870	0.54
08/31/1998	135	10.8	90.3	800	0.50
11/10/1998	145	5.1	90.7	600	0.38
02/09/1999	159	7.7	90.1	700	0.44
04/19/1999	169	5.0	NA	290	0.19
04/21/1999	169	6.4	NA	700	0.44
04/22/1999	169	6.4	NA	705	0.44

Humidity and Air Pressure in the Heated Drift

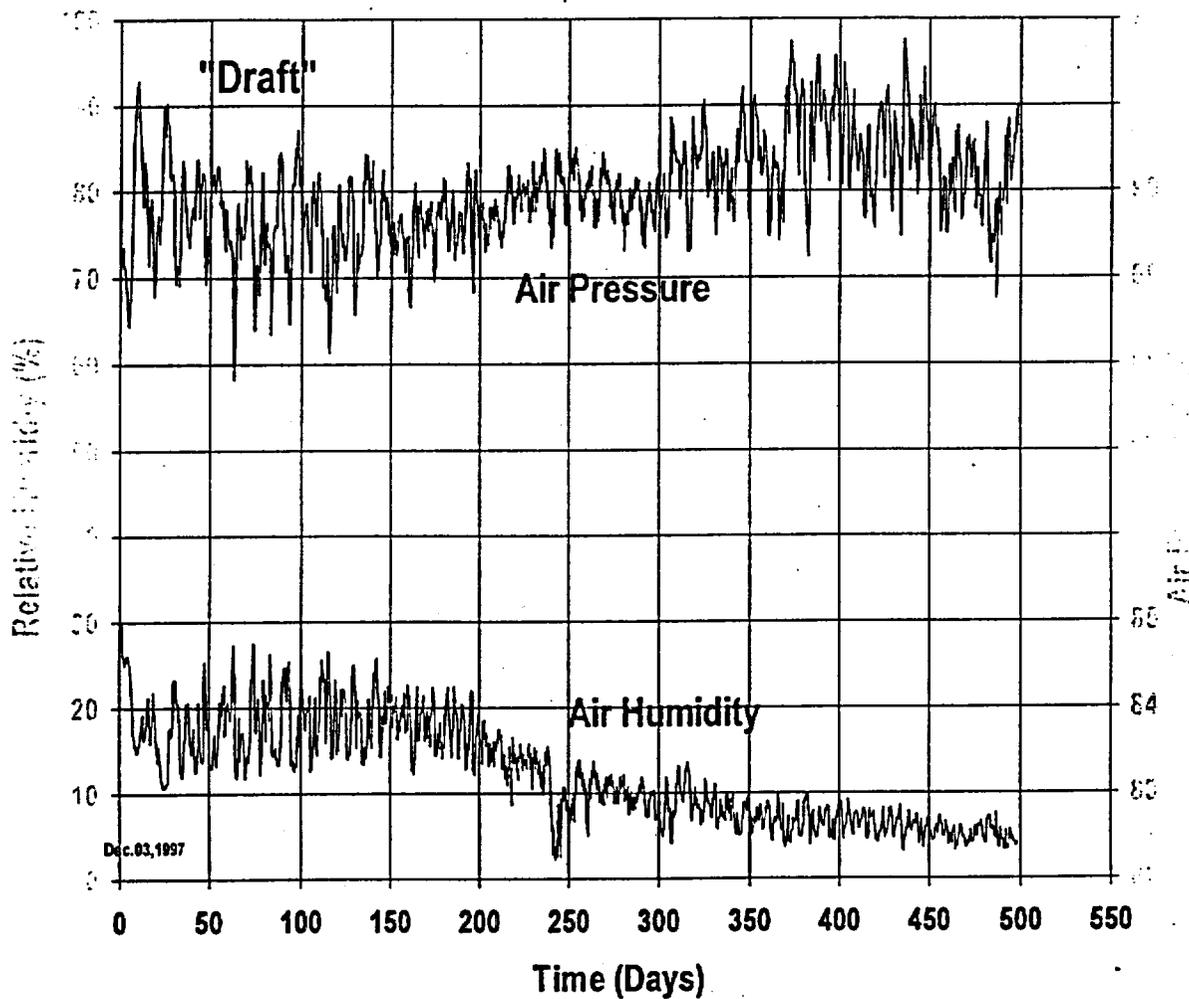


Figure 3.11-1 Inverse relationship of barometric pressure and relative humidity in heated drift.

Location	Heat Flux (W/m ²)			
	05-Jan-99	23-Mar-99	26-Apr-99a	26-Apr-99b
1	242	296	277	300
2	344	310	316	338
3	425	594	541	519
4	360	721	699	744
5	592	767	821	823
Est. Total Conductive Heat Loss (kW)	5.1	7.0	6.9	7.1

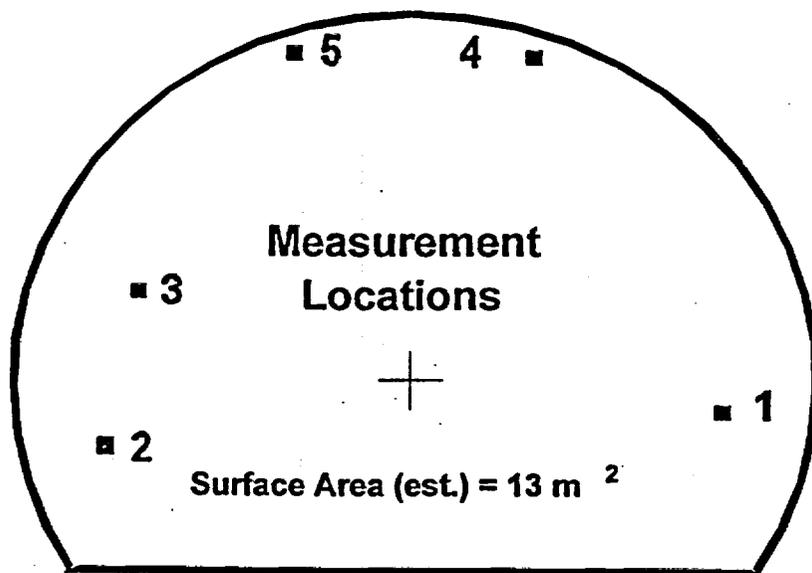


Figure 3.11-2 Measured convective loss on the bulkhead.

DOE/NRC APPENDIX 7 MEETING ON THERMAL TESTING
Las Vegas, Nevada

April 28, 1999

Description of Meeting/Attendees

On April 28, 1999, staff from the U.S. Nuclear Regulatory Commission (NRC) and the U.S. Department of Energy (DOE) conducted an Appendix 7 Meeting in Room 302 of the DOE Facilities at the Hillshire Bldg., Summerlin, Las Vegas to discuss thermal testing associated with the Drift Scale Test (DST). Participants included representatives from the NRC, the Advisory Council on Nuclear Waste (ACNW), the Center for Nuclear Waste Regulatory Analysis (CNWRA), the DOE Yucca Mountain Site Characterization Office (YMSCO), the Nuclear Waste Technical Review Board (NWTRB), and staff from the YMSCO Civilian Radioactive Waste Management System (CRWMS) Management & Operating contractor and Management and Technical Services contractor. The NRC technical lead was Brett Leslie. The DOE technical lead was Deborah Barr (U.S. Bureau of Reclamation (USBR)/DOE). No other stakeholders were represented. The agenda and the list of attendees are included in the records package and available electronically.

Presentation/Discussion Overview

D. Barr (USBR/DOE) and B. Leslie (NRC) made brief introductory remarks.

Unconstrained heat and mass loss through bulkhead and via ventilation and its impact on interpretation of results

J. Pohle (NRC) introduced the first topic: Unconstrained heat and mass loss through bulkhead and via ventilation and its impact on interpretation of results.

R. Green (CNWRA) presented a discussion on simulation modeling he had done using an analog scale model of a heated drift. Green noted that he would like to see monitoring of the amount of vapor and air escaping around the bulkhead in the DST. At this time, DOE does not have a good handle on how much mass is moving around the bulkhead. Green did note that with the repository design switch to Enhanced Design Alternative-2 (EDA2) some of his concerns went away (e.g., air pressure build up, as there will not be as much build up with the cooler design of EDA-2). At present the DST is not designed to detect dripping. R. Wagner (M&O) noted that the DST is overdriving the system six to eight times the heating compared to EDA-2 and three to four times the Viability Assessment (VA) repository design. This would suggest that there will be no dripping until the cool-down phase. W. Lin (LLNL) noted that the location of drips will be apparent when we go back into the DST. R. Datta (M&O) also noted that the camera could detect any dripping. Green indicated that in his model, the drips were caustic and actually destroyed the detectors. D. Wilder (LLNL) noted that this is not a good analog for the chemistry of the site as a concrete liner is no longer planned. Green agreed that the caustic chemistry was due to the concrete liner in the model. D. Barr (USBR/DOE) asked if the fractures in the model are realistic when considering the scale of the model. Green indicated the fractures were not to scale. Barr suggested that the scale of the fractures in the model would be a feature in the repository from which we would have a stand-off distance, and thus dripping from these features would not be a concern. Wagner noted that sporadic testing of vapor and air outflow around the

bulkhead may not get an accurate picture. Green agreed, the outflow varies over time due to barometric pressure and other considerations. There should be constant monitoring.

D. Hughson (CNWRA) presented a discussion on her computer simulation modeling of the DST. The presentation was a reiteration of much of what was in the recent CNWRA report that she published with Green. The model was a dual-continuum model with a two-dimensional grid, smeared heat load and a horizontal temperature distribution.

R. Wagner presented a discussion on a Recap of Events and Activities regarding the heat and mass loss through the bulkhead.

T. Buschek (LLNL) presented a discussion on the impact on modeling. Much of this presentation was similar to that which was presented the day before in the thermal testing workshop. R. Datta noted that measuring heat on both sides of bulkhead will give more data. R. Wagner indicated that conductive heat loss was okay, the problem is convective heat loss. D. Barr noted that when considering any changes to the test, we have to differentiate between what would be nice to have and what is essential to have. We need to determine what we can live with considering the budget. D. Wilder suggested that we need to balance the value of data lost versus decreasing uncertainty. There may also be cost savings associated with test changes. For example, it may cost initially to install insulation to reduce heat loss but this may mean that less electricity is needed to heat the DST to the required temperature. T. Buschek noted that not much money is going to analyze the results of the test. B. Leslie emphasized that they were trying to get across the NRC concerns regarding the test; it is up to the DOE to decide what to do. D. Wilder asked whether, with EDA-2 now being preferred design and the DST being planned to look at the old proposed design, the Project should consider changing DST to bring it more in line with EDA-2. R. Datta suggested that this might be accomplished by shutting off the wing heaters.

Y. Tsang (Lawrence Berkeley National Laboratory [LBNL]) presented a discussion on the Effect of Heat and Moisture Loss Through the Bulkhead on the Interpretation of Results of the Drift Scale Test. Tsang noted that whether the heated drift bulkhead is considered an open or closed boundary does not affect the utility of the DST in evaluating the coupled thermal-hydrologic processes. The uncertainties in evaluating the bulkhead as a closed or open boundary are small compared to other uncertainties, such as heterogeneity. As an example of heterogeneity, Tsang cited fracture permeability, which can vary by three orders of magnitude and uses a geometric mean as a representative value. She noted that in two similar boreholes different temperatures were recorded. This is probably due to different fracture permeability in the holes. W. Lin suggested that water loss may affect coupon testing in DST. T. Buschek noted that some water was also lost due to initial ventilation. D. Wilder noted that the system is not sealed, and he asked whether, if you had a sealed system, more water would go into the rock? Buschek indicated more water would go into the rock and that water would not remain in the drift during the heating period, so the coupon test is all right as it is.

Discussion: R. Datta (M&O) began the discussion period by noting that he could not find a gage capable of measuring the small fluctuations necessary to assemble a convection monitoring method. R. Green suggested that redundant calibrated manometers can measure this. B. Leslie indicated that information on a supplier could be provided and Green volunteered to send this information via e-mail to Datta. Datta suggested that the Project has a good handle on what is going on at the bulkhead. To verify the amount of convective loss, the Project needs a monitoring system to assess air flow, temperature, and humidity. B. Leslie suggested that old

ventilation data may provide some early or confirmatory data for air flow that passed the bulkhead.

How are thermal-mechanical results being used to support repository design, and what additional thermal-mechanical data from other repository units will be collected to support repository design?

B. Jagannath (NRC) introduced the next topic and introduced A. Ghosh (CNWRA) who provided a presentation on some concerns with the testing. The concerns involved:

- prediction of thermal-mechanical response observed at thermal tests
- applicability of the measurements to the proposed repository horizon as the measurements are being made in the middle non-lithophysal while 75% of the proposed repository horizon is in the lower lithophysal
- sufficiency of the thermal-mechanical data gathered for the repository horizon
- effects of alternative designs and how results from the tests are being incorporated into design.

Observation: The order of the Yucca Mountain Project personnel presentations was altered from the proposed agenda to allow a presentation on the data to be first.

R. Finley (M&O, Sandia National Laboratories) presented a discussion on The Available Data from the Tests. Finley noted that for the Single Heater Test, the final report contains much more data.

R. Wagner provided a presentation on additional Thermal-mechanical Data From Other Units. Wagner noted that whether or not the cross-drift thermal test is done or not depends upon the budget. D. Wilder stated that the design the Project is currently considering is different from the DST. This difference could be a driver for the cross-drift test. Wilder asked if this had been factored into the cross-drift proposal. Wagner indicated it hadn't, that much more planning is needed for the final proposal.

Rick Nolting (M&O, Repository Subsurface Design) provided a presentation on The Use of Thermal Test Thermal-mechanical Data by Repository Design. Nolting noted that any tests in the cross drift will be for performance verification after license application. A. Ghosh asked how in situ results are used versus lab results. Nolting indicated that the Project will use range-bounding values for design values.

W. Lin (M&O, LLNL; Note: Lin presented rather than D. Wilder who was listed on the agenda) provided a presentation on the Thermal-mechanical-hydrological Modeling in the Near-field Process Model Report.

Discussion: B. Jagannath suggested that another Appendix 7 meeting be held before the DOE finalizes plans for the Lower Lithophysal characterization. B. Leslie noted that the NRC does not get data in a timely fashion. He suggested that the principal investigators should check with Bill Boyle (DOE), as there may be a way to allow NRC to get the data quicker through some of the protocols for the International Decovelex.

Water and gas sampling protocols and flow of information to and from Performance Assessment

B. Leslie (NRC) introduced the concerns on this topic and noted that a focus should be placed on performance. What does Performance Assessment (PA) require? What are the constituents that control degradation? Predictions can't be made in PA unless we have constrained data. The primary user of data is PA. Leslie also raised the question of whether the sampling protocols are sufficient.

L. DeLoach (M&O, LLNL) provided a presentation on Aqueous Sampling and Chemistry in the Drift Scale Test. DeLoach noted that the Seamist system did not work as originally anticipated. B. Leslie asked if there was a work package that described the procedure. DeLoach answered that there was, but she thought the procedure was skimpy. She went to the field and observed the implementation of the procedure. She then wrote a more detailed procedure and may need to revise the procedure again to make it more detailed. It may be necessary to have the data taken by someone more knowledgeable. She also noted that the Seamist system was experimental. Some parameters are hard to sample for minimizing atmospheric exposure. Leslie suggested getting rid of the eight meters of hose. DeLoach stated that that is in the new protocol. Leslie noted that there are other methods that can be used. J Pohle (NRC) queried what is basis for tests. DeLoach answered that volume was. R. Wagner noted that this is an evolving issue; as the Project goes along and gains more experience, the procedure is revised. Leslie noted that the neutron holes have water in them and asked whether someone samples this water when the holes are logged. D. Barr stated that the chemistry is "screwy" in these holes due to concrete and other things (grouting, Teflon, etc.) in the neutron holes. R Datta said that the Project is considering converting chemistry holes. Y. Tsang said that the Project will convert chemistry/Seamist holes to two packed-off hydrology holes. Leslie indicated this would be great and asked if this will be permanently installed. Tsang answered yes. The Project will be doing this with lowermost chemistry holes.

E. Sonnenthal (M&O, Lawrence Berkeley National Laboratory) provided a presentation on Modeling of Thermal-hydrological-chemical Behavior. He discussed the pore waters and gas chemistries that could seep into the drifts. B. Leslie asked how sensitive fluoride is and whether it can tell you the fracture interaction. Sonnenthal said that it may give a fracture/matrix interaction. Different species may help provide estimates, especially the species U^{234}/U^{238} . Sonnenthal discussed that the model used is a dual permeability model incorporating mineralogy and aqueous species. M. Hamura (SNL) asked why PCO_2 is so small in model near the heater. D. Sassani (M&O) indicated that this was due to fractures being open and ventilation.

N. Francis (SNL) provided a presentation on Performance Assessment Operations Thermal-hydrological and Coupled Processes. R. Wagner asked Francis to detail flow of data to PA. B. Leslie said this was not necessary, that it was now clear on how the information flows to PA.

B. Leslie made closing remarks to state that he appreciated everyone's efforts and that this meeting was a very positive experience.

Assessment of meeting effectiveness

Based on Leslie's closing statement meeting was very effective in providing information to the NRC and addressing their concerns.

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Enclosure 4

5 Pages

Commitments

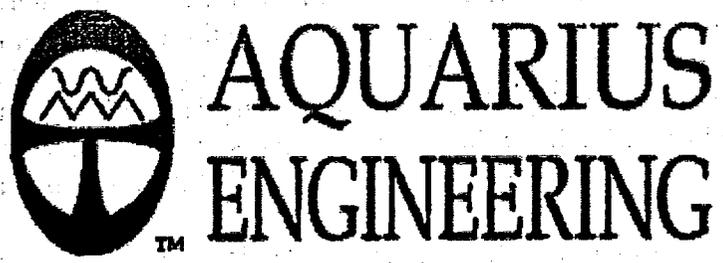
No commitments are made at Appendix 7 meetings.

Observations

No additional observations were made beyond those discussed above.

New Issues/Concerns/Recommendations

None were noted.



home

**Written Comments to the Public Meetings of the U.S.N.R.C. Advisory
Committee on Nuclear Waste, June 1999, San Antonio, TX, and the U.S.
Nuclear Waste Technical Review Board, June 1999, Beatty NV**

*Submitted by Donald L. Baker, Ph.D. Soil Physics
Aquarius Engineering
2000 West Maine Street
Fayetteville AR 72701-6257*

"And our method of breaking this down was, in fact, to take a drop of water and walk it through the mountain, and a drop of water in a rain cloud until it hits a receptor -- what happens to it, physically and in a process manner as it walks through the mountain" -- Mr. Jack Bailey, Director of Regulatory and Licensing for the M&O operating contractor at YMP, from the transcript of the 105th Meeting of the Advisory Committee on Nuclear Waste, Dec 16, 1998, Rockville MD.

These remarkable powers of observation fall short of noting the fall of every sparrow on two counts. First, the scientifically accepted methods for doing so are several approximations removed from reality. A real soil is approximated by an ideal soil, which is approximated by analytic equations, which are approximated by numerical methods. At each step the process is simplified so that it is both easier for mortals to calculate and comprehend, and thus subject to additional errors. Second, the people who do this have not yet taken account of all the errors, even in the lowest, numerical step. And worse, even when presented with the math, those in areas of responsibility at National Laboratories deny that they exist.

Here follows excerpts from a recent unsolicited proposal to the National Science Foundation, with enough equations and references to raise doubts among any with the will to follow the math:

The Development of Darcian Means for Models of Unsaturated Ground Water Flow

*Donald L. Baker, Ph.D. Soil Physics
Principal Investigator*

Introduction and Justifications

The storage and fate of underground nuclear waste and other hazardous materials is about to become a bigger can of worms than previously thought. First, the plutonium is moving, likely attached to moving soil colloids. According to Kersting, et al. (1999), the plutonium produced by nuclear tests at the Nevada Test Site has not waited upon the disposition of those who made it. It has been found in well water a mile south from at least one large 1968 blast, in a climate perhaps chosen for its lack of rainfall. This makes it all the more critical to use the best available methods to predict its movements.

Second, new work (Baker, 1999c) has demonstrated that existing models of unsaturated water flow, which commonly use standard means, such as the arithmetic mean, for interblock hydraulic conductivity means, may contain unaccounted errors in non-Darcian flow. Indeed, the arithmetic mean can be shown by both mathematics and modeling in many circumstances to be entirely non-physical, producing significant flow errors even for very small space steps.

Until now, it has been generally assumed that mass-conservative methods, such as the modified Picard method (Celia, et al., 1990), for modeling Richards' unsaturated flow equation [1], along with adaptive gridding and time steps, meet all such needs. Indeed, the paper by Celia, et al., claim for the method reduction of the time step discretization error along with "perfect" mass balance. Although this is a significant contribution to the state of the art, the more recent work of the P.I. demonstrates that mass conservation alone does not account for all sources of modeling error.

$$[1] \frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x} \left[K(h) \cdot \frac{\partial H}{\partial x} \right], \text{ where } \theta = \text{volumetric water content (cm}^3/\text{cm}^3), t = \text{time (s), } x = \text{position or gravity potential head (cm, positive upwards), } K(h) = \text{unsaturated hydraulic conductivity (cm/s), } H = \text{total head (cm)} = h + x, h = \text{hydraulic pressure head (cm).}$$

Baker (1995a) has demonstrated that the modified Picard method does indeed suffer from time-step discretization error, which can be reduced by higher-order Runge-Kutta methods and adaptive time stepping, separately and in combination (Baker, et al., 1998b, unpublished, available at the web site cited below). Warrick (1991) demonstrated that standard interblock hydraulic conductivity means in numerical models of [1] did not conform to the modeling assumptions of constant flow [2] between grid points (Figure 1) and Darcy's law [3]. Warrick found the non-Darcian flows generated by standard means of $K(h)$ such as the arithmetic mean to be as much as two orders of magnitude in error.

$$[2] \frac{\partial q}{\partial x} = 0, \text{ where } q = \text{unsaturated flux density (cm/s).}$$

$$[3] q = -K(h) \cdot \frac{\partial H}{\partial x} = -K(h) \cdot \frac{\partial(h+x)}{\partial x}$$

The integral form used by Warrick did not work well for all soils and conductivity relations when it required integrating through a discontinuity. Baker (1994, 1995b) recast the approach as an elliptic boundary condition problem [4], which was more generally applicable. In this approach, [4] is solved on a super-fine grid between x_1 and x_2 shown in Figure 1 with a tri-diagonal numerical method. The boundary conditions are taken to be the matric suction (negative pressure) heads, ψ_1 and ψ_2 .

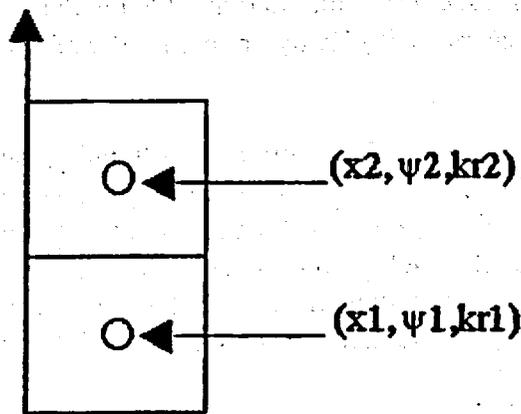


Figure 1: Adjacent vertical grid cells, centered at x_1 and x_2 , with matrix suction ψ and relative conductivity k_r .

$$[4] -\frac{\partial q}{\partial x} = \frac{\partial}{\partial x} \left[K(\psi) \cdot \frac{\partial H}{\partial x} \right] = \frac{\partial}{\partial x} \left[K(\psi) \cdot \frac{\partial (x - \psi)}{\partial x} \right] = 0$$

When the flow between super-fine grid cells is constant to a given percentage of flow between x_1 and x_2 , the iteration is stopped. The resulting Darcian mean interblock conductivity, k_m , is calculated from the constant flow, q , and the difference form of the head gradient [5]. This solution is only good between these two grid centers and for the period of one time step in the larger model. The solution must change when the grid center suction heads, ψ_1 and ψ_2 , are updated in the next time step.

$$[5] q = -k_m \cdot \frac{\Delta H}{\Delta x}$$

While this method rests on the assumption of constant flow, q , between grid points, Baker (1999c) also recognized another unbiased Darcian mean. It depends only upon Darcy's law, the distribution of K with respect to x in physical fine-grid wetting front, and the unsaturated hydraulic conductivity relation $K(\psi)$. Suppose that q in [5] is the integral mean with space, x , in [6]. It can then be related to the discrete form of Darcy's law [5], using the mean flow and mean conductivity. The continuum form of Darcy's law [3] can be integrated as in [7], and related to [6] through the mean flow. Setting [6] and [7] equal through the mean flow, we can solve for the unbiased Darcian mean conductivity, K_v , in [8].

$$[6] \bar{q} = \frac{1}{\Delta x} \cdot \int q dx = -\bar{K} \cdot \frac{\Delta x - \Delta \psi}{\Delta x}$$

$$[7] \int q dx = -\int K dx + \int K d\psi$$

$$[8] K_v = \frac{\Delta x \cdot K_x - \Delta \psi \cdot K_h}{\Delta x - \Delta \psi}, \quad K_x = \frac{1}{\Delta x} \cdot \int K(x) dx, \quad K_h = \frac{1}{\Delta \psi} \cdot \int K(\psi) d\psi$$

If one runs a very-fine-grid model of vertical infiltration into very dry soil, one can integrate the distribution of $K(x)$ over x and $K(\psi)$ over ψ from the numerical results of the wetting front profile at particular times to obtain K_v as a function of grid point values of K or ψ , and the vertical displacement,

Δx . For the range of the study in Baker (1999c), k_m (called K_d in the study) agreed with K_v within 2%. By contrast, the arithmetic mean disagrees with K_v by up to an order of magnitude. Additional results are discussed later.

Both of these methods of solution are practical only for investigating the nature of Darcian means, not for actually solving [1]. They are higher-order approximations than assuming that the properties of a grid cell are constant throughout the cell, which produces the harmonic mean, and the assumption that relative conductivity is linear from x_1 to x_2 , which produces the arithmetic mean. The k_m -approach [4] allows the head and relative conductivity to vary nonlinearly with distance between x_1 and x_2 so that [2] and [3] are preserved. Baker (1998a) investigated the nature of this kind of relation in depth for several types of unsaturated conductivity relations.

Drs. Liu and Bodvarsson of Lawrence Berkeley National Laboratory appear to be centrally involved in the characterization modeling of Yucca Mountain (Bodvarsson, et al., 1997). Because the models and data are held secret under the Q clearance, it is difficult to tell what methods are actually being used. But their criticism of the very nature of Darcian means gives a solid indication that the errors due to non-Darcian flow from standard means are not considered or accounted in such modeling.

A letter from J. Russell Dyer, Project Manager, Yucca Mountain Site Characterization Office, dated Jan 05, 1999, contained a review of Baker (1998a) and other works (Baker, et al., 1998b,c) by Drs. Liu and Bodvarsson. They have, for example, misapplied a trivial case to suggest that Darcian means are invalid in the case of "a 1D, vertical, steady-state flow system with a constant infiltration at the top boundary", and thus inappropriate in general. But in homogeneous soil, for which Darcian means have thus far been developed, this is only the case of gravity flow, where the pressure head, h , is constant and the flow is driven entirely by the gravity head, x .

Consider the unsteady infiltration problem [9], using infiltration of water into a typical fracture in Topopah Spring welded tuff at Yucca Mountain, after Schenker, et al., (1995) and Baker (1998a). Figure 2 shows the conductivity state space of the preceding model, the diagram of every pair of adjacent points in the model on the basis of hydraulic conductivity values. There are 4000 pairs of (K_1, K_2) , where K_2 is the conductivity of the grid point immediately above the K_1 position. At the initial condition of the model (Init State), 3966 pairs sit at one spot in the lower-left-hand corner. The rest are distributed according to the initial condition equation in [9], mostly in the upper-right-hand corner, close to the $K_1=K_2$ diagonal. At the end of a model run (End State), the pairs are distributed with only 528 remaining at their starting points in the lower-left-hand corner. The other 3472 pairs have moved in arcs through the state space to come increasingly close to the $K_1=K_2$ diagonal.

Solve equation: $\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x} \left[K \frac{\partial H}{\partial x} \right]$, $H = \psi - x_d$, x_d positive downwards,

ψ = matric suction (negative pressure head)

Boundary conditions: $\psi(0,t) = 0.082m$, $K(0.01m,t) = 4.74(10^{-11})m/s$, $10^{-7} \leq t \leq 10^{-3} s$

$$[9] \text{ Initial conditions: } K(x,0) = \begin{cases} 0.0474 - 0.1766493x_d / \sqrt{t} & , x_d < 8.49(10^{-5})m \\ 4.74(10^{-11}) & , 8.49(10^{-5})m \leq x_d \leq 0.01m \end{cases}$$

Saturation relation: $\theta(\psi) = 1.084(10^{-4}) + 2.6414(10^{-3}) \cdot (\psi / 0.082m)^{-0.739}$, $\psi \geq 0.082m$

Conductivity relation: $K(\psi) = 4.74(10^{-3}) \cdot (\psi / 0.082m)^{-8.875}$, $\psi \geq 0.082m$

Adaptive numerical time step: Δt chosen so that mass balance is maintained to one part in 10^8 or better in 10 or less iterations.

In this diagram, the points above the $K1=K2$ -axis represent wet-over-dry conditions; below is dry-over-wet. Darcian or any other kind of means form the third dimension above the plane, a contour surface of $K_{mean}(K1,K2)$. The contour surfaces of all possibly valid means must pass through the $K1=K2$ diagonal, or they will not be mathematically valid. Because of this, all possibly valid means approach the same limit on the diagonal, $K_{mean} = K1 = K2$, and thus approach each other. This is why all possibly valid means produce convergence to the fine grid solution. But this necessary condition does not guarantee, as has been shown in Baker (1999c) with the arithmetic mean, that all such means are physically valid. If a mean is not mathematically valid, it cannot be physically valid.

If the upper boundary condition and initial conditions had been set at the inflow and through flow of $4.74(10^{-11})$ m/s, a steady-state condition would have resulted, with all the 4000 pairs remaining at one point in the lower-left-hand corner, namely $(K1, K2) = (\log(4.74(10^{-11})), \log(4.74(10^{-11})))$. Thus the case cited by Liu and Bodvarsson is but a single point in the plane on the $K1=K2$ -axis, a rather trivial case. Since all valid possible means, even poor ones, pass through such a point, it cannot be invoked to demonstrate invalidity.

And when using a steady flow upper boundary condition, one simply adjusts the grid slightly and replaces the topmost flow that was calculated by a Darcian mean with the flow boundary condition. Conductivity means are not usually relevant to use as a flow boundary condition. Replacing a mean with an upper flow boundary condition leaves the remaining means below it just as valid as they were before, even more so if they are trivial cases. Thus, Liu and Bodvarsson argue a moot if not specious point.

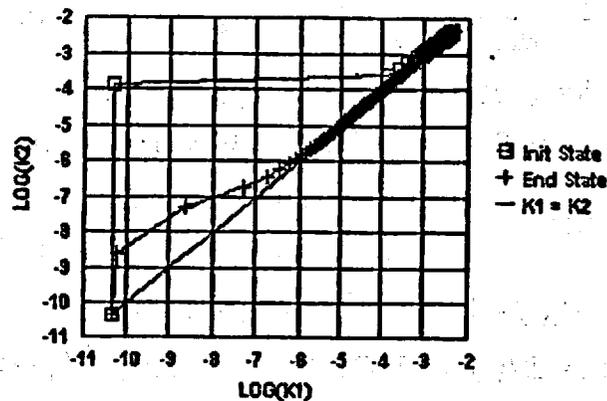


Figure 2: Conductivity State Space Diagram for [9]

Init State at $t = 10^{-7}$ s. End state at $t = 10^{-3}$ s

The cited work with Darcian means suggests that as one moves from the $kr_1=kr_2$ axis (relative conductivity version of $K_1=K_2$), standard means, such as the arithmetic, geometric, harmonic or upstream, which are independent of soil unsaturated hydraulic properties, produce flow that are increasingly non-Darcian, in violation of the assumptions [2] and [3]. Liu and Bodvarsson (communication cited above) suggest, without proof or example, that the differences are so small that they can be adequately addressed by adaptive gridding. However, Baker, et al. (1999a) show that as vertical grid spacing increases, using the arithmetic mean loses up to 50% of the mass infiltrated at fine grid spacings. A Darcian mean approximation can reduce this error to 0.5%. In addition, Baker (1999b) shows significant ratio differences near the $kr_1=kr_2$ -axis between true and approximate Darcian means, and the arithmetic and geometric means, for average fracture and matrix media flow (Schenker, et al., 1995), respectively, in Topopah Spring welded volcanic tuff at Yucca Mountain.

Later work (Baker, 1999c) solves [9] with very fine to coarse grids to demonstrate the non-Darcian flow errors of the arithmetic mean in very small space steps. This work also demonstrated that for very small space steps Darcian means for Brooks-Corey conductivity relations can be collapsed into 2-D plots, where the independent variable is K_1/K_2 . As noted above, all valid interblock means approach each other as K_1 approaches K_2 , and can produce more severely non-Darcian flow away from that condition.

So it is legitimate to consider how a model of [9] behaves when each pair of points at least begins each time step with a constant ratio of K_1/K_2 across the wetting front. This was done with the three different interblock means for a constant-ratio distribution of 8, 10, 12, 16, 20, 24, 28, 38, 66, 124, 240 and 470 points across the wetting front from $t = 10^{-7}$ to $t = 10^{-3}$ s. The arithmetic mean and two approximations to Darcian means were used, as in [9], but with up to 40 iterations per time step. At the end of each time step, the grid was adjusted back to a constant ratio of adjacent grid point conductivities.

Figure 3 shows the end-of-run results for a model of [9] using the arithmetic mean, K_a . The arithmetic mean has no relation to either the hydraulic properties of the porous medium or the vertical space step size of the model. The wetting front profiles for 8, 10, 12, 16, 20, 14, 28, 38 and 470 point pairs, n , in the wetting front show a classical convergence to the fine-grid solution on the left. On the right, the solution for 8 pairs overestimates the position of the leading edge of the wetting front by 18.75%.

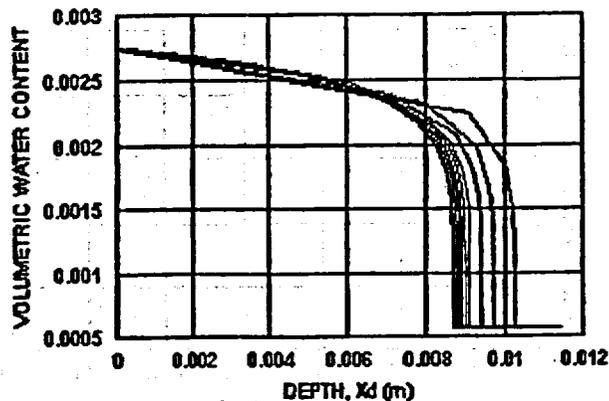


Figure 3: Wetting Fronts for K_a and $n = 8, 10, 12, 16, 20, 24, 28, 38$ and 470

The plot for $n = 470$ is on the left, and the others approach it as n increases

Figure 4 shows the results for an approximate Darcian mean, K_h , that accounts for the porous medium hydraulic conductivity parameters, but not the model vertical space step size. For $n = 8, 10, 12, 16$ and 470 , the wetting front profiles converge from a position -3.40% behind the fine-grid solution to the fine-grid solution. Figure 5 shows the results for an approximate Darcian mean, K_{dim} , that accounts for both the conductivity parameters and the model vertical space step size, with $n = 8, 10, 12$ and 470 . In all the runs from $n = 8$ to $n = 470$, with an additional run at $n = 48$, the estimated position of the wetting front varied from -0.18% to $+0.36\%$ with this mean. This is the same order of magnitude as the error associated with adjusting the grid spacing after each time step. When the maximum errors are considered over the range of conductivity ratios, the ratio is $52.1:9.4:1$ for $K_a:K_h:K_{dim}$.

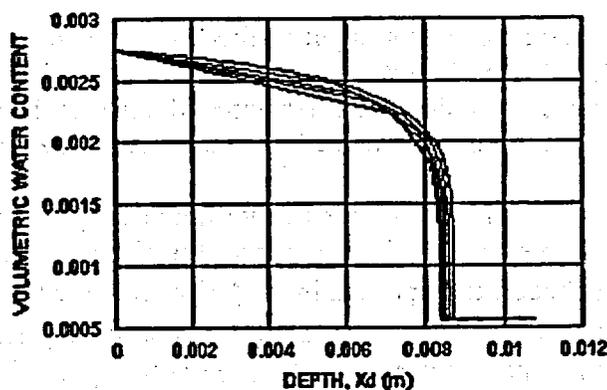


Figure 4: Wetting Fronts for K_h and $n = 8, 10, 12, 16$ and 470 (470 on the right)

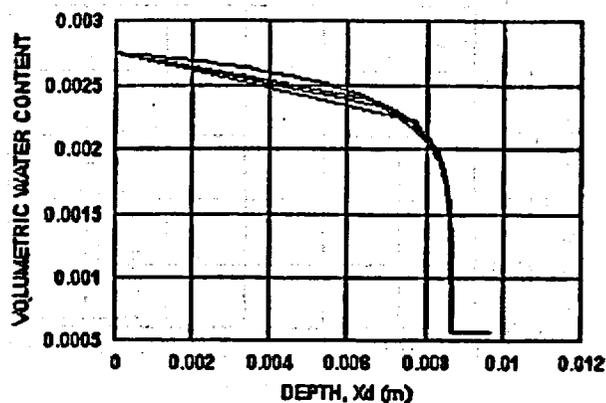


Figure 5: Wetting Fronts for K_{dim} and $n = 8, 10, 12$ and 470

One can, of course, pick a grid spacing that shows the arithmetic mean in a much more favorable light. If one spaces uniform grid points along the wetting front profile, the segments with the largest flows will have the smallest conductivity ratios (for adjacent points). The segments with the smallest flows will have conductivity ratios many orders of magnitude higher, producing larger errors in the smaller flows at the leading edge of the wetting front.

Above a certain number of grid points, it may seem as if the flow errors are self-compensating. But they are still there and unaccounted. If the criterion for environmental impact is the time of arrival of a waste front in parts-per-billion, how can one guarantee it with unaccounted flow errors? These errors are orders of magnitude larger than the once-famous Pentium division bug. The scientific responsibility for their accounting rests not on he who demonstrates their existence, but on those who claim they are insignificant without actually having calculated their effects.

We have seen what happens when the onus was put on the Morton-Thiokol Engineers to demonstrate the negative, that the launch of the Space Shuttle SRB would not be safe with cold o-rings. And now we have evidence that the plutonium does not wait upon the dictates of any established agenda. It moves. And when it arrives, it will have a much greater impact than a Space Shuttle falling out of the sky.

As the cited literature demonstrates, Darcian means vary dramatically and nonlinearly with both soil properties and vertical space step size, especially as space step size passes through the equivalent air displacement length, ψd . This becomes important in models of fracture flow, where the average model vertical space step size may be much larger than ψd . And it is becoming more apparent that the transport of soil colloids through fractures may be very important to the transport of nuclear waste products.

The Darcian mean approach may be the logical key to understanding why some standard interblock conductivity means have been found to work best with particular soils in certain regimes. It now offers to modelers a new modeling and mathematical framework with which to judge the appropriateness of their approximations of interblock conductivity means for unsaturated flow. It extends the validity of models in conductivity state space farther from the $kr_1=kr_2$ -axis, and may offer new criteria for deciding how adaptive gridding should be done. When developed with higher-order adaptive time steps (Baker, et al., 1998b) and adaptive grids, Darcian means may offer a new order of magnitude of computational efficiency due to their higher accuracy, but this remains to be developed and demonstrated.

Proposed Work

This section of the proposal is proprietary and confidential. It may not be used for any purpose other than the internal review of the National Science Foundation.

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Some Questions for the Modelers of Unsaturated Flow and Transport for the Yucca Mountain Project, Hanford Tank Initiative, Nevada Test Site and other DOE Programs.

Submitted by
Donald L. Baker, Ph.D. Soil Physics
Aquarius Engineering
2000 West Maine Street
Fayetteville, AR 72701
www.aquarinen.com
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Summary

Recent work (publications and draft papers on www.aquarinen.com) in numerical methods for modeling the vertical unsaturated flow of water in porous media has uncovered previously unrecognized errors in standard methods. These errors may affect the validity and reliability of models that attempt to predict the flow of water and the transport of hazardous and nuclear waste on the scale of tens to thousands of years. The following questions and three-point grid test demonstrate how the common arithmetic mean of intergrid unsaturated hydraulic conductivity violates Darcy's law for vertical unsaturated flow in all but a few trivial conditions, and can even violate the mathematical minimum-maximum principle for elliptic boundary value problems (steady-state flow problems). By contrast, a Darcian intergrid conductivity mean for the exponential pressure-conductivity relation solves such problems perfectly. The numerical examples in the appendix compare parallel models of a relaxing wet pulse in a long, vertical fracture, using the exponential pressure-conductivity relation. One model uses the arithmetic mean, and the other the analytic Darcian mean, with exactly the same adaptive time steps for both. The arithmetic mean model exhibits a dry spike that grows with the logarithm of time, and oscillations similar to numerical dispersion, both associated with space steps where the arithmetic mean can violate the min-max principle. By contrast, the Darcian mean model is smooth and well-behaved.

Some Questions on Model Validity

Would you agree that it is necessary for a modeler of unsaturated flow to be cognizant of all the sources and relative magnitudes of error in his or her numerical calculations? Would you agree that this allows a modeler to construct a variable or adaptive grid so as to produce the least error? If not, make an irrefutable scientific argument for the contrary view.

Would you agree that any method of calculating steady-state unsaturated flow would be both physically and mathematically invalid if it violated either the minimum-maximum principle for elliptic boundary value problems (D.W. Zachmann & P. DuChateau, 1986, Schaum's Outline Series, Theory and Problems of Partial Differential Equations, pp 19-21) or Darcy's law? If not, can you give a scientific justification for your answer that is beyond all refutation?

Would you contend that any such method that commits either of these violations in a model of steady-state flow is then valid to use in a model of transient flow? If so, can you give a scientific justification for your answer that is beyond all refutation?

Would you agree that any method that commits one or both of these violations would be inappropriate to use in models designed to predict and assure the safety of a nuclear waste site over the scale of thousands of years? If not, can you give a scientific justification for your answer that is beyond refutation?

Can you demonstrate that all the methods that you use for calculating unsaturated flow in your models do not violate either the min-max principle or Darcy's law in any case or regime in which your models are used? If not, can you give a scientific justification that is beyond all refutation for why your models should be considered to be valid and reliable?

Do you recognize equation [1] as Darcy's law in the finite form and [2] as Darcy's law in the continuum form?

$$[1] \bar{q} = -K_s \cdot K_v \cdot \frac{\Delta H}{\Delta x} = -K_s \cdot K_v \cdot \frac{\Delta x - \Delta \psi}{\Delta x}, \text{ where } \bar{q}\text{-bar (m/s) is the mean mass flow across}$$

the vertical distance, Δx (m), K_s (m/s) is saturated hydraulic conductivity, K_v is the mean relative hydraulic conductivity across vertical Δx , and ΔH (m) is the total hydraulic head difference across Δx , where $H = x - \psi$, x (m) is the vertical position or head and ψ (m) is the matric suction (or negative pressure) head.

$$[2] q = -K(\psi) \cdot \frac{\partial H}{\partial x} = -K(\psi) \cdot \frac{\partial x - \partial \psi}{\partial x}$$

Consider the three-point system of steady-state, constant, vertical, unsaturated flow in a homogeneous porous medium in Figure 1, with fixed boundary conditions $\psi_2(x_2)$ and $\psi_0(x_0)$, where $x_0 = 0$, $x_1 = \Delta x$ and $x_2 = 2 \cdot \Delta x$ in the vertical. Let K_m be the estimate of unsaturated hydraulic relative conductivity mean between x_0 and x_2 , and k_{m1} and k_{m2} be the estimates by the same method between x_0 and x_1 , and x_1 and x_2 , respectively. Let H_0 , H_1 and H_2 be the total heads at x_0 , x_1 and x_2 , such that $H_0 = -\psi_0$, $H_1 = \Delta x - \psi_1$ and $H_2 = 2 \cdot \Delta x - \psi_2$. Would you agree that equation [3] is an accurate and valid application of Darcy's law in [1] in this case?

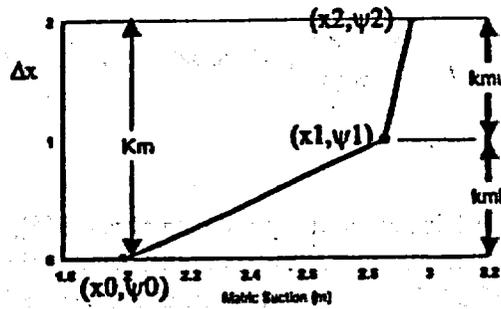


Figure 1: Three-Point System of Steady-State Flow

$$[3] \frac{-q \cdot \Delta x}{K_s} = K_m \cdot (H_2 - H_0) / 2 = k_{ml} \cdot (H_1 - H_0) = k_{mu} \cdot (H_2 - H_1)$$

If one solves the two right-hand-sides of [3] against $K_m \cdot (H_2 - H_0)$ for H_1 , sets them equal and divides out common terms of $(H_2 - H_0)$, the result is then equation [4]. Would you agree that in order to satisfy Darcy's law and calculate the same constant flow on both the Δx and $2 \cdot \Delta x$ scales, that any method to estimate the intergrid conductivity means, K_m , k_{ml} and k_{mu} , would also have to satisfy equation [4]? And would you agree that if it failed to satisfy equation [4] that this would raise a legitimate question as to its validity in a model of unsaturated flow? If not, please demonstrate mathematically why not.

$$[4] K_m = \frac{2 \cdot k_{ml} \cdot k_{mu}}{k_{ml} + k_{mu}}$$

Suppose that the method in question is the arithmetic mean, such that $K_m = (k_{r0} + k_{r2})/2$, $k_{ml} = (k_{r0} + k_{r1})/2$ and $k_{mu} = (k_{r1} + k_{r2})/2$, where $k_{r0} = k_r(\psi_0)$, $k_{r1} = k_r(\psi_1)$, $k_{r2} = k_r(\psi_2)$ and $k_r(\psi)$ is the unsaturated relative conductivity relation for the porous medium in Figure 1. Substitute the arithmetic means for k_{ml} and k_{mu} into equation [3] and cancel common terms, like 2. Would you agree that equation [5] is a valid result and the only unknown in the equation is ψ_1 , which can be solved by iteration or Newton's method? Equations [4] and [5] are both derived from equation [3]. Would you agree that the value of $k_{r1} = k_r(\psi_1)$ resulting from [5] determines the values of k_{ml} and k_{mu} , and that substituting them back into equation [4] is a reasonable way to check the mathematical and physical validity of the arithmetic mean, or any other method of estimation?

$$[5] (k_r(\psi_1) + k_{r2}) \cdot (H_2 - \Delta x + \psi_1) - (k_{r0} + k_r(\psi_1)) \cdot (\Delta x - \psi_1 - H_0) = 0$$

Consider a porous medium where the unsaturated conductivity relation is determined by equation [6], with $\eta = 8.1$ and $\psi_d = 0.08$ m. Given the expected values published in Schenker, et al. (1995, Stochastic hydrogeological unites and hydrogeological properties development for total-system performance assessments, Sandia Report SAND94-0244*UC-814 under DOE contract DE-AC04-94AL85000), is this a reasonable possible expression for the relative conductivity of a fracture in Topopah Spring welded volcanic tuff, if one uses a Mualem or Burdine transformation to derive $k_r(\psi)$ from the pressure-saturation parameters given in Schenker, et al? If not, can you specify a more correct set of η and ψ_d parameters to use in this example?

$$[6] \quad k(\psi) = \begin{cases} 1 & , \psi \leq \psi_d \\ (\psi_d / \psi)^\eta & , \psi > \psi_d \end{cases}, \text{ where } \psi_d = \text{"displacement pressure" head (m) and } \eta \text{ is a fitting parameter.}$$

Please verify that Table 1 is the set of solutions to equation [5], given equation [6], with $\psi_d = 0.08$ and η as given in column 2. Is it not apparent from this table that for $\eta = 8.1$ the arithmetic mean produces a value of ψ_1 that violates the min-max principle for any Δx greater than about 0.50366 m? It is possible to show that the arithmetic mean satisfies both equations [4] and [5] in the trivial case of pure gravity flow, where $\psi_0 = \psi_1 = \psi_2$. But is it not apparent from Table 1 that the arithmetic mean fails satisfy Darcy's law in steady state flow for $\psi_0 \neq \psi_2$ and $\Delta x > 0.50366$ m? Is it not also apparent that the arithmetic mean likely violates the min-max principle for $\eta = 2.1$ and 4 and for $\Delta x > 0.80422$ and 0.56667 m, respectively? If you do not agree, can you demonstrate the opposite mathematically?

Table 1: Solutions to Figure 1 with the Arithmetic Mean

The variables η , Δx , ψ_0 , ψ_1 and ψ_2 are as described above. The variable, ψ_1 , is determined by the solution to equation [5], $k_1 = k(\psi_1) = (0.08/\psi_1)^\eta$, $k_{m1} = (k_0 + k_1)/2$, $k_{m2} = (k_1 + k_2)/2$, $K_m = (k_0 + k_2)/2$ and the mean of means is $2 \cdot k_{m1} \cdot k_{m2} / (k_{m1} + k_{m2})$, the right-hand-side of equation [4]. The ψ_1 column tests conformity to the min-max principle, that ψ_1 is included in the range $[\psi_0, \psi_2]$. Rows 8 and 9 show violation of the min-max principle. Rows 1, 2 and 7 show the boundary of violation for the min-max principle. The last two columns on the right test the balance of equation [4] for the arithmetic mean, which fails in every row.

	η	Δx (m)	ψ_0 (m)	ψ_1 (m)	ψ_2 (m)	k_1	k_{m1}	k_{m2}	K_m	mean of means rhs of [4]
1	2.1	0.80422	0.5	1	1	.004972	.013142	.004972	.013142	.007214
2	4.0	0.56667	0.5	1	1	4.1e-5	.000348	4.1e-5	.000348	7.33e-5
3	8.1	0.001	0.5	0.58860	1	9.54e-8	2.26e-7	4.83e-8	1.79e-7	7.97e-8
4	8.1	0.01	0.5	0.59200	1	9.11e-8	2.24e-7	4.62e-8	1.79e-7	7.66e-8
5	8.1	0.1	0.5	0.63450	1	5.11e-8	2.05e-7	2.66e-7	1.79e-7	4.71e-8
6	8.1	0.5	0.5	0.99634	1	1.34e-9	1.79e-7	1.32e-9	1.79e-7	2.63e-9
7	8.1	0.50366	0.5	1	1	1.3e-9	1.79e-7	1.3e-9	1.79e-7	2.59e-9
8	8.1	1	0.5	1.494	1	5.0e-11	1.79e-7	6.8e-10	1.79e-7	1.35e-9
9	8.1	2	0.5	2.4873	1	8.1e-13	1.79e-7	6.5e-10	1.79e-7	1.3e-9

Consider again equations [4] and [5], which derive from Darcy's law for steady-state flow that is constant in space in equation [3]. Is it not apparent from these equations that a method of estimating an intergrid hydraulic conductivity mean that upholds Darcy's law must contain an accounting for the model vertical space step term, Δx ?

It may be possible that the non-Darcian flow errors generated by the arithmetic mean are small enough to make it of practical use in some modeling regimes. Can you provide a mathematical

justification for when this would be the case? Can your justification account for both the pressure-conductivity relation, $kr(\psi)$, and the model vertical space step size, Δx ?

If you are using some other method of estimating the intergrid hydraulic conductivity mean in your models, can you perform this analysis and demonstrate that any other method you use does not produce similar violations of Darcy's law and the min-max principle?

If not, would you agree that a method that did account for both $kr(\psi)$ and Δx , and did not violate either Darcy's law or the min-max principle would be more appropriate for use in both models of steady-state and transient flow?

Do you again recognize equation [2] as the continuum form of Darcy's law? Consider that if kr is a function of ψ and ψ is a function of x , then kr is also a function of x . Do you recognize equation [7] as the expression of flow that is constant in space, and equation [8] ([7] applied to [2]) as the expression of steady-state flow that is constant in space and time, as long as the boundary conditions are constant in time? If the conductivity relation and its inverse are as described in [9], please verify that [9] and the spatial distribution of $kr(x)$ in [10] satisfy [8].

$$[7] -\frac{\partial(q / K_s)}{\partial x} = 0$$

$$[8] \frac{\partial}{\partial x} \left[kr(\psi(x)) \cdot \frac{\partial}{\partial x} (x - \psi(x)) \right] = \frac{\partial kr(x)}{\partial x} \cdot \left[1 - \frac{\partial \psi(x)}{\partial x} \right] - kr(x) \cdot \frac{\partial^2 \psi}{\partial x^2} = 0, \text{ where the}$$

boundary conditions are $(x_1=0, \psi_1)$ lower and $(x_2=\Delta x, \psi_2)$ upper and constant in time, which may also be expressed as $(0, kr_1=kr(\psi_1))$ and $(\Delta x, kr_2=kr(\psi_2))$.

$$[9] kr(x) = \exp(\eta \cdot (\psi_d - \psi(x))), \quad \psi(x) = \psi_d - \ln(kr(x)) / \eta$$

$$[10] kr(x) = a \cdot \exp(-\eta \cdot x) + b, \quad a = \frac{kr_1 - kr_2}{1 - \exp(-\eta \cdot \Delta x)}, \quad b = \frac{kr_2 - kr_1 \cdot \exp(-\eta \cdot \Delta x)}{1 - \exp(-\eta \cdot \Delta x)}$$

Equation [11] is [1] rewritten. Equation [12] is the integration of [2], allowing that $kr(\psi(x))$ can also be expressed as $kr(x)$. Do you recognize [13] and its implication as a legitimate definition of mean flow in a problem [8] where the flow is constant in time and space, and the resulting value of K_v as the legitimate definition of a mean intergrid hydraulic conductivity in that problem? Please verify that substituting [9] and [10] into the definition of K_v in [13] produces the expression in [14].

$$[11] -\bar{q} \cdot \Delta x / K_s = K_v \cdot (\Delta x - \Delta \psi)$$

$$[12] -\frac{1}{K_s} \int q dx = \int kr(x) dx - \int kr(\psi) d\psi$$

$$[13] \bar{q} = \frac{1}{\Delta x} \int q dx \Rightarrow K_v = \frac{\int kr(x) dx - \int kr(\psi) d\psi}{\Delta x - \Delta \psi}$$

$$[14] K_v = \frac{u \cdot (kr_2 - kr_1 \cdot e^{-u})}{(1 - e^{-u}) \cdot (u - \ln(kr_1 / kr_2))}, \quad u = \eta \cdot \Delta x$$

Since K_v is derived from the analytic solution to the steady-state problem in equation [8], it is called a Darcian mean. Do you see that this approach depends intimately on the pressure-

conductivity relation, $kr(\psi)$, in [9]? Please verify that as $kr1$ goes to $kr2$, Kv goes to $Kv = kr1 = kr2$, that as Δx goes to zero, Kv goes to $(kr1 - kr2)/\ln(kr1/kr2)$ and that as Δx goes to +infinity, Kv goes to $kr2$. Note that the first limit perfectly predicts that when $\psi0 = \psi2$ in the case of pure gravity flow, that $\psi0 = \psi1 = \psi2$.

Let Kv be expressed as a function $Kv(kr1, kr2, \Delta x)$. Referring to the problem in Figure 1 and equations [3] and [4], let $Km = Kv(kr0, kr2, 2 \cdot \Delta x)$, $kml = Kv(kr0, kr1, \Delta x)$ and $kmu = Kv(kr1, kr2, \Delta x)$. The result, using the exponential conductivity relation in [9] is shown in Table 2. (Note: The exponential conductivity relation in [9] is used here instead of the Brooks-Corey relation in [6] because there is as yet no explicit analytic solution for Kv with [6]. But the results of using the arithmetic mean with an exponential $kr(\psi)$ are much the same character as in Table 1.) In every row of Table 2, the min-max principle is preserved and equation [4] is balanced. Is it not apparent that the Darcian mean represents not just the estimate of the mean necessary to solve the problem in Figure 1, given the conductivity relation in [9], but the true mean that perfectly satisfies Darcy's law in this case?

Table 2: Solutions to Figure 1 with a Darcian Mean

The variables η , Δx , $\psi0$, $\psi1$ and $\psi2$ are as described above. The variable, $\psi1$, is determined by the solution to equation [5], $kr1 = kr(\psi1) = \exp(\eta(\psi0 - \psi1))$, $kml = Kv(kr0, kr1, \Delta x)$, $kmu = Kv(kr1, kr2, \Delta x)$, $Km = Kv(kr0, kr2, 2 \cdot \Delta x)$ and the mean of means is $2 \cdot kml \cdot kmu / (kml + kmu)$, the right-hand-side of equation [4]. The $\psi1$ column tests conformity to the min-max principle, that $\psi1$ is included in the range $[\psi0, \psi2]$. The last two columns on the right test the balance of equation [4]. In each case, the min-max principle and Darcy's law are perfectly preserved.

	η	Δx (m)	$\psi0$ (m)	$y1$ (m)	$y2$ (m)	$kr1$	kml	kmu	Km	mean of means rhs of [4]
1	2.1	0.80422	0.5	0.87887	1	0.1868	0.2259	0.1594	0.1964	0.1964
2	4.0	0.56667	0.5	0.88249	1	0.0404	0.0722	0.0296	0.0420	0.0420
3	8.1	0.001	0.5	0.58392	1	0.0169	0.0242	0.0048	0.0080	0.0080
4	8.1	0.01	0.5	0.58836	1	0.0163	0.0237	0.0046	0.0077	0.0077
5	8.1	0.1	0.5	0.64069	1	0.0107	0.0184	0.0029	0.0050	0.0050
6	8.1	0.5	0.5	0.91656	1	0.0011	0.0034	6.8e-4	0.0011	0.0011
7	8.1	0.50366	0.5	0.91831	1	0.0011	0.0034	6.8e-4	0.0011	0.0011
8	8.1	1	0.5	0.99790	1	5.9e-4	0.0012	5.8e-4	7.7e-4	7.7e-4
9	8.1	2	0.5	0.999	1	5.8e-4	7.7e-4	5.8e-4	6.6e-4	6.6e-4

If you do not agree, please offer the proof, consisting of a set of conditions and numerical values for which Kv either violates the min-max principle or Darcy's law using [3] and [4]. Please explain under what valid scientific principle the YMP modelers at the DOE Lawrence Berkeley National Laboratory may claim that this approach to calculating intergrid hydraulic conductivity means is not physically based and cannot be valid in the gravity flow case where $\psi0 = \psi1 = \psi2$. Please extend that argument to explain why one cannot take any other conductivity relation, such as [6], solve the elliptic boundary value problem [8] numerically, and thus obtain $kr(x)$ and a valid numerical value for Kv . Is it not apparent that this approach for develops Darcian means for

steady-state flow? If you disagree, can you demonstrate that it will produce a worse answers in numerical transient flow models than commonly-used means, such as the arithmetic mean, that do not account for $k_r(\psi)$ or Δx , and occasionally violate the min-max principle?

In the finite method expression [15] of Richards' equation for unsaturated flow in a homogeneous medium, modelers sometimes make separate calculations for the intergrid hydraulic conductivity means for gravity (advective), K_x , and capillary (diffusive) flow, K_ψ . This may be justified by using [13], as in [16], redefining the integrals as the respective mean conductivities, K_x and K_ψ , over Δx and $\Delta \psi$ [17]. But notice that in general it is difficult, if not impossible, to know the spatial distribution, $k_r(x)$, between grid points in a transient flow problem. It is common to calculate the integral that defines K_ψ , but to substitute a much simpler mean, such as the arithmetic mean, for K_x . Notice the effect that such a substitution in [16] has on the mathematically equivalent [15], since K_v can now be defined as in [18]. Near hydrostatic conditions, Δx goes to $\Delta \psi$, and K_v in [18] suffers from division by zero, producing a singularity with limits at infinity, if K_x and K_ψ are not perfectly related through the derivations of Darcian means presented here. Can you certify that you do not use any such method in your models? If you do, can you provide mathematical proof that the errors generated by the singularity are not significant in every case?

$$[15] \theta_i^{j+1} = \theta_i^j + r \cdot [K_{v_{i+1/2}} \cdot (H_{i+1} - H_i) - K_{v_{i-1/2}} \cdot (H_i - H_{i-1})], \quad r = K_s \cdot \Delta t / \Delta x^2$$

[16]

$$\theta_i^{j+1} = \theta_i^j + r \cdot \left[\frac{K_x \Delta x - K_\psi \Delta \psi}{\Delta x - \Delta \psi} \Big|_{i+1/2} (\Delta x - \Delta \psi) \Big|_{i+1/2} - \frac{K_x \Delta x - K_\psi \Delta \psi}{\Delta x - \Delta \psi} \Big|_{i-1/2} (\Delta x - \Delta \psi) \Big|_{i-1/2} \right]$$

$$= \theta_i^j + \frac{\Delta t \cdot K_s}{\Delta x} (K_{x_{i+1/2}} - K_{x_{i-1/2}}) - r \cdot [K_{\psi_{i+1/2}} \cdot (\psi_{i+1} - \psi_i) - K_{\psi_{i-1/2}} \cdot (\psi_i - \psi_{i-1})]$$

$$[17] K_x = \frac{1}{\Delta x} \cdot \int k_r(x) dx, \quad K_\psi = \frac{1}{\Delta \psi} \cdot \int k_r(\psi) d\psi$$

$$[18] K_v = \frac{K_x \cdot \Delta x - K_\psi \cdot \Delta \psi}{\Delta x - \Delta \psi}$$

What is the difference between determining that an error is tolerable and denying that it even exists? Is it logical and legitimate to say that a "carefully designed grid system" eliminates an error that one claims does not exist? Is it possible that carefully accounting for all the errors is a prerequisite for designing a grid system? And finally, if one scientist has a calculator, and another can show that for even one case the calculator gives back 2.5 for 1+1, which scientist has the responsibility to demonstrate the practical usefulness and validity of the calculator in all cases?

Appendix: Numerical Examples - Parallel Models of a Relaxing Wet Pulse Using the Arithmetic and Darcian Means (excerpts from a paper in progress)

Now consider a numerical experiment for a long, vertical, homogeneous fracture described by pressure-conductivity relation [9] and the pressure-saturation relation [19], using parameters, $K_s = 0.00474$ m/s, $\eta = 6.4$ (1/m), $\psi_d = 0.08$ m, $\theta_s = 1$, $\theta_r = 0.0395$ and $\beta = 0.64$ (1/m). These

conductivity parameters very crudely model an average fracture in Topopah Spring welded volcanic tuff (Schenker, et al., 1995), with the saturation parameters chosen simply and arbitrarily to keep count of mass balance. A fracture of depth, $x_l = 512$ m, is modeled with a finite difference form of the Richards' unsaturated flow equation [15], using the modified Picard method (Celia, et al., 1990) with an adaptive time step (Baker, et al., 1998). In this case, just to make x equal to depth, x will be positive downwards. The upper boundary will be a matric suction (2.95823 m) such that $kr = 10^{-3}$. The lower boundary is no-flow and set up such that the depth, x_l , is constant no matter how many grid points, 0 to np , in the model.

$$[19] \frac{\theta - \theta_r}{\theta_s - \theta_r} = \begin{cases} 1 & , \psi \leq \psi_d \\ \exp(\beta \cdot (\psi_d - \psi)) & , \psi > \psi_d \end{cases}, \text{ where } \theta = \text{volumetric water content} \\ (\text{m}^3/\text{m}^3, \text{ effectively dimensionless}) \theta_r = \text{residual water content, } \theta_s = \text{saturated water} \\ \text{content, and } \beta \text{ and } \psi_d \text{ are fitting parameters}$$

The initial condition of all the grid points in the model will be a matric suction such that $kr = 10^{-3}$, except for the points from $0.35 \cdot x_l$ to $0.45 \cdot x_l$, which shall be set to a positive pressure head of 1 m ($\psi = -1$ m). The number of points, np , in model will be an even multiple of 10, such as, 40, 60, 100, 140, 200, 280, 400, giving space steps of $\Delta x = 12.8, 8.533, 5.12, 3.657, 2.56, 1.829$ and 1.28 m for $x_l = 512$ m. (Note: The same errors occur in smaller reaches, but the large-scale plots make the dispersive nature of some oscillations more apparent.)

Because the mass inflow and outflow at the boundaries of this experiment will be orders of magnitude smaller than the mass flow in the interior, the relative global mass balance, as defined by Celia, et al., will not be used. Instead, each time step will be calculated to converge to an error, rmb , in the equivalent depth of water of 10^{-10} m. The error, $rmb = \text{sumth} - \text{flx}$, where

$\text{sumth} = \frac{\Delta x}{2} \cdot \sum_{i=1}^{np} (\theta'_{i-1} - \theta'_{i-1} + \theta'_{i+1} - \theta'_i)$ is the trapezoidal integral of the mass change in the model during one time step, and $\text{flx} = -K_{m/2} \cdot (H_1 - H_0) \cdot \Delta t / \Delta x$ is the mass flow into the upper boundary of the model in one time step. $K_{m/2}$ is the intergrid hydraulic conductivity mean between the $x_0 = 0$ upper boundary and the first grid point at $x_1 = \Delta x$.

In this case, two models will be run in parallel for comparison. One uses the arithmetic mean, K_a , for the intergrid conductivity mean. The other uses the Darcian mean in [14], K_v . The model using the Darcian mean will be set to adjust the time steps so that it converges to $rmb < 10^{-10}$ m in 40 iterations or less. The model using the arithmetic mean will use exactly the same time steps, but will be allowed to converge in 80 iterations or less. If the either model does not converge in the allotted number of iterations, then the time step is reset and reduced, and both models are rerun for that time step. If the Darcian mean model converges in less than 40 iterations, the time step is increased slightly. The maximum time step is limited to $5(10^5)$ s. In this way, any difference between the two models involving time step as well as space step discretization error is removed. Both are equally affected.

Figure 2a shows the results for the arithmetic mean model for $np = 40$, $\Delta x = 12.8$ m, at $t = 0, 10, 0.512(10^6), 1.024(10^6), 2.048(10^6)$ and $4.096(10^6)$ s. Figure 2b shows the results in the same run for the Darcian mean model. Note the different vertical scales, necessary due to radically different responses. This is the model of an initial-condition pressure pulse that should be both relaxing and drifting downwards in the fracture. In the first ten seconds, the arithmetic mean model produces excess negative matric suction (positive pressure) heads that are non-physical.

The Darcian mean model, by contrast, relaxes completely to the just under saturation near a matric suction of 0.08 m, with no apparent change in pulse shape.

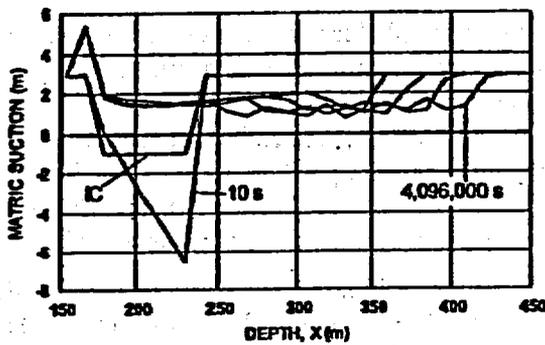


Figure 2a: Arithmetic Mean Model
Initial pulse of $y = -1$ m between $0.35x_l$ and $0.45x_l$, relaxing and translating with time, for $n_p = 40$ at $t = 0, 10, 0.512(10^6), 1.024(10^6), 2.048(10^6)$ and $4.096(10^6)$ s, in the example fracture

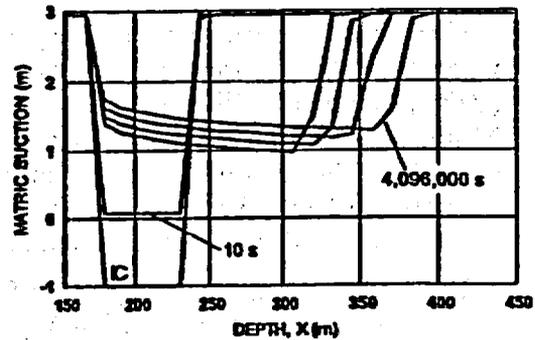


Figure 2b: Darcian Mean Model
for $n_p = 40$ running in parallel with the same time steps in the same fracture and the same output times.

As the models progress, the arithmetic mean model develops a persistent non-physical spike in matric suction at the top edge of the pulse (left on graph). This is a direct result of violation of the min-max principle, as demonstrated in the three-point grid test in the questions above. The arithmetic mean model also develops severe oscillations in the peak of the pulse, producing many non-physical peaks that are consistent with the concept of mass clumping due to a differential error in hydraulic conductivity between wet-over-dry and dry-over-wet conditions. By contrast, the Darcian mean model is very smooth and well-behaved.

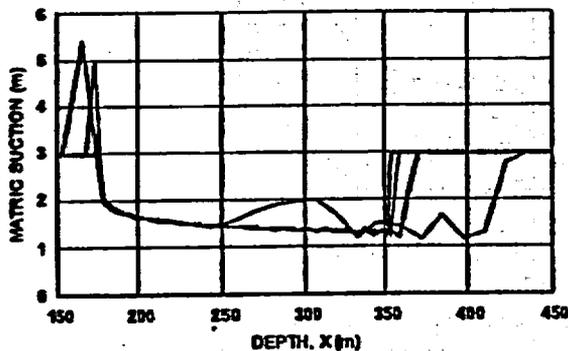


Figure 3a: Arithmetic Mean Model
Convergence to the fine-grid solution, for $n_p = 40, 100, 200$ and 400 , or $\Delta x = 12.8, 5.12, 2.56$ and 1.28 m.

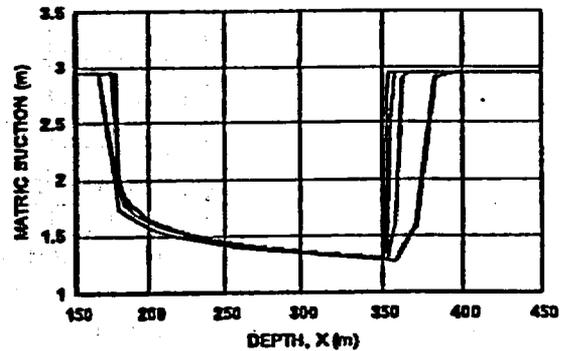


Figure 3b: Darcian Mean Model
Convergence to the fine-grid solution, for $n_p = 40, 100, 200$ and 400 , or $\Delta x = 12.8, 5.12, 2.56$ and 1.28 m. Parallel time step run with Arithmetic mean model.

Figures 3a and b show the convergence of the arithmetic mean and Darcian mean models for $n_p = 40, 100, 200$ and 400 , or $\Delta x = 12.8, 5.12, 2.56$ and 1.28 m, at $t = 4.096(10^6)$ s. As step size goes down, the trailing edge suction spike and the leading edge oscillations in the arithmetic mean model decrease. Both models converge to the same fine-grid solution, but the Darcian mean model shows superior error and stability characteristics.

Non-Darcian flow errors are not apparent in this example for vertical space step sizes below where the arithmetic mean actually violates the min-max principle. But in another example (Baker, 1999b), of infiltration into a fracture to less than 1 cm, with space steps from 1.5 mm to 21 μm , and an adaptive grid set to maintain a constant ratio between adjacent grid conductivities, using the arithmetic mean produced errors in the wetting front position of up to 18.75%, compared to 0.36% for an approximate Darcian mean. It may be that non-Darcian flow errors are tolerable in many cases, but this cannot be certified unless they are actually accounted.

The oscillations in the leading edge of the pulse in the arithmetic mean model are reminiscent of numerical dispersion in hyperbolic systems. But classical numerical dispersion is created by the differing speeds of propagation of different frequency components of the pulse. Here the differing speeds of propagation are generated directly by errors in the intergrid conductivity mean, and depend as well on the slope of the pulse. This kind of oscillation has been seen previously in fracture flow infiltration using a van-Genuchten-style conductivity relation in Baker, et al. (1999a).

Figure 4 shows how the matric suction spike evolves as a function of time and model vertical space step size, Δx . The trend, out to 83,886,100 s in model time, is for the non-physical spike to increase logarithmically in time, once it starts to develop. The plot for $n_p = 40, \Delta x = 12.8$ m, is atypical, possibly because of increasing space step discretization error. Note that the plots for 1.829 and 2.56 m start to decrease before rising above the initial conditions behind the pulse. The reasons for delayed onset and the apparent logarithmic increase of the dry spike are not fully understood at this time.

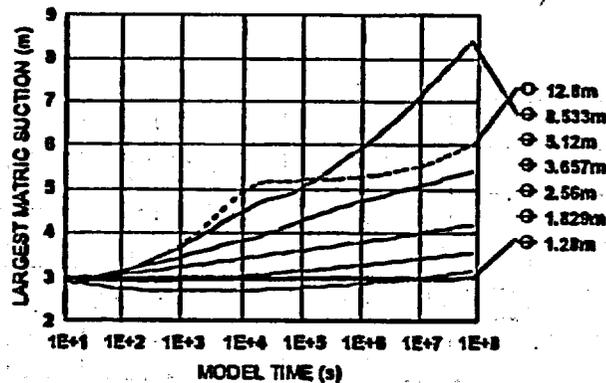


Figure 4: Trailing Edge Matric Suction Spike for arithmetic mean model for $n_p = 40, 60, 100, 140, 200, 280$ and $400, \Delta x = 12.8$ to 1.28 m; The grid point with the largest spike value at $t = 8.39(10^8)$ s is tracked from $t = 10$ to $8.39(10^8)$ s.

Although it does not show well, note that even for $n_p = 400, \Delta x = 1.28$ m, the grid point at the trailing edge of the initial pulse rises from the initial condition of 2.95823 m to 2.99623 m at the end of the run. There is no physical reason for it to do so; the gravity flow into the fracture is the

same as in the fracture to the top edge of the relaxing pulse. If the pulse were diffusing upwards, the trend would be in the opposite direction. If the pulse had reached the no-flow lower boundary and the fracture were filling with water, due to the upper boundary inflow of $4.74(10^{-10})$ m/s, the trend would be in the opposite direction. The model end time is about 2.63 years, and the non-physical spike for the $\Delta x = 1.28$ m case is just beginning to show. This does not bode well for models that use the arithmetic mean, or any other significantly non-Darcian mean in violation of the min-max principle, to predict flow over scales of thousands of years.

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Office of Civilian Radioactive Waste Management

The Control and Use of Scientific Notebooks for OCRWM Activities



QA98005, Revision 2

M&O Training & Development

Class Overview

Objectives

Origin of SN Control

SN Importance

SN General Principles

SN Identification & Control

SN Planning

SN Initial Entry

SN In-Process Entries

SN Review & Approval

Data Submittal

SN Closure

Records

Lessons Learned

Summary

Notes

Objectives

Upon completion of this lesson, each participant will understand the process to initiate, develop, review, and process Scientific Notebooks

SCIENTIFIC
NOTEBOOK



Notes

Scientific Notebook (SN)—A record of the planning, methodology, requirements, and results of scientific investigations that is used when the work involves a high degree of professional judgment or trial and error methods, or both.

SN Compliance Review—A review of a scientific notebook using a defined checklist for the compliance of AP-SIII.1Q and QA procedures listed in Section 7.0 of this procedure, except for the technical review component of the checklist.

SN Entry—Information recorded in a scientific notebook for activities performed over the duration, usually each day, of activity. (Any number of entries may be made on any given day in a single scientific notebook by any number of Investigators who initial and date each of their entries.)

SN Register—A Lotus Notes database used to track all Yucca Mountain Site Characterization Project scientific notebooks, including a unique identifier, responsible individual, title, and review tracking capabilities.

SN Supplemental Record—A record, created while conducting the work covered by a scientific notebook, that cannot be conveniently included in the scientific notebook, such as computer listings, floppy disks, magnetic tapes, large volume supplementary explanatory materials, or large plots.

Technical Reviewer—An individual assigned to provide a technical review who has not performed the work to be reviewed and is qualified to retrace the described work, to confirm the results or repeat the work and achieve comparable results without recourse to the original investigator.

Objectives

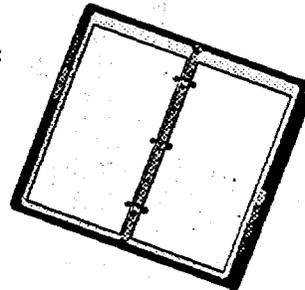
- Describe the process for initiating a SN
- Define the review requirements for a SN
- Describe the data submittal requirements
- Describe the closeout and submittal process for a SN



Notes

Origin of SN Control

- > QARD
 - > III.2.2, Performing Scientific Investigations
 - * Use of SN
 - * SN contents
 - * SN reviews
 - > AP-SIII.1Q, Scientific Notebooks
 - * Identification and control
 - * Entries & reviews
 - * Submittal of data
 - * Closure
 - > NRC Expectations

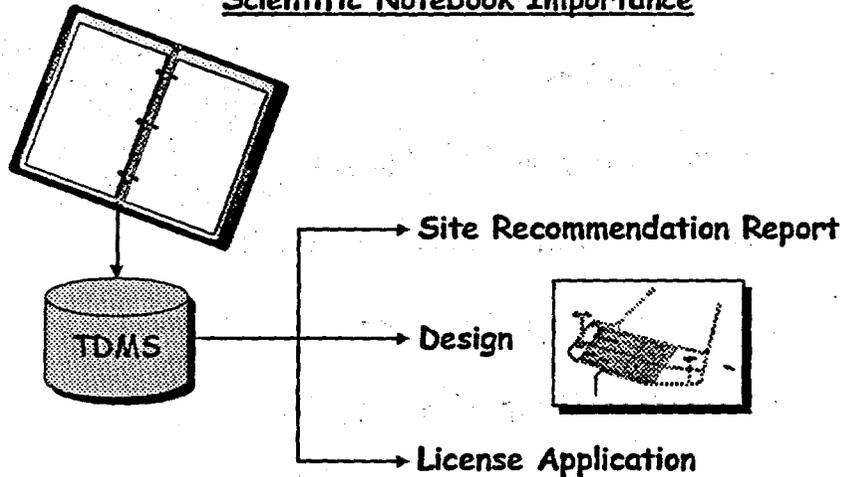


Notes

AP-SIII.1Q, Scientific Notebooks establishes the process and responsibilities for the documentation of scientific investigations that involve a high degree of professional judgement or trial and error methods, or both, in scientific notebooks when implementing procedures are not appropriate. The procedure does not apply to the conduct of repetitious processes and activities, but may be used to support such activities.

This procedure applies to individuals with the Management and Operating Contractor (M&O), including the national laboratories, and to the U.S. Geological Survey that use scientific notebooks for activities subject to the U.S. Department of Energy Office of Civilian Radioactive Waste Management *Quality Assurance Requirements and Description*, DOE/RW-0333P. Scientific notebooks initiated under another approved procedure must be transitioned to this procedure, with an entry signifying transition within 45 work days of the effective date of this procedure.

Scientific Notebook Importance



Notes

Scientific Notebook Importance

- Begins a chain-of-custody for scientific information
- Provides the inputs, and in some cases, the foundation for higher-level documents

Technical Databases

Site Recommendation Report

Requirements documents

Design

License Application

- Must be documented and reviewed correctly to ensure regulator confidence in our scientific process and determinations

Scientific Notebook General Principles

- Bound/Binders
- Consecutively numbered pages
- Permanently attach loose materials
- Avoid excessive blank space
- Reference all supplementary records
- Initial or sign, and date entries



Scientific Notebook General Principles

Notes

1. Scientific investigations shall be performed using scientific notebooks, implementing documents, or a combination of both.
2. Unless otherwise approved by the manager of the investigator using the scientific notebook and documented in the initial entry, a bound notebook with consecutively numbered pages shall be used. If a three-ringed binder or equivalent is used, all pages also must be consecutively numbered and each entry dated.
3. When incorporating loose materials, permanently attach the materials in the scientific notebooks.
4. Avoid excessive blank space that has no purpose in scientific notebooks. Blank pages or substantial blank space on a page shall be identified for future purpose such as a table of contents, a log of referenced documents, or other reserved purpose. Blank spaces, indentation, or other format options used to improve readability do not need to be labeled. At closure of the notebook, draw a diagonal line through all areas where the reason for the existence of the open space is not otherwise obvious; then initial and date the slash.
5. Reference all applicable scientific notebook supplementary records of supporting information created while conducting the work, but which cannot be conveniently included in the scientific notebook, such as review documentation.
6. Initial or sign, and date entries on the day they were made. Entries should be made on the date the work was performed unless it is more appropriate or descriptive to consolidate an overlapping, ongoing event or process.

Scientific Notebook General Principles

- Corrections and legibility
- Security
- Table of contents
- Clear, concise, complete statements
- Failed experiments are important



Notes

Scientific Notebook General Principles

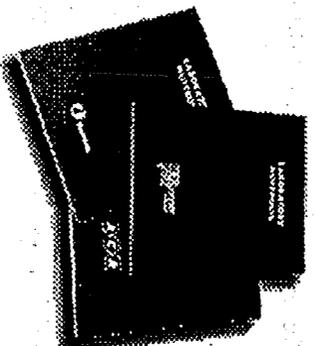
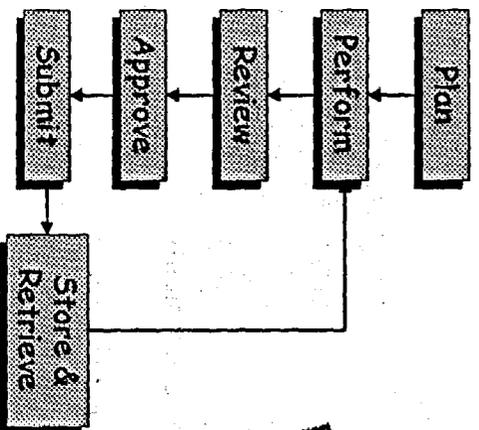
7. Make and date corrections to scientific notebook entries or supporting information by drawing a single dark line through the incorrect or obliterated information and placing the correct information or explanation, including an explanation of the obliteration, in close proximity, or note another location where the information is documented. Ensure that scientific notebook entries, including corrections, are sufficiently legible for imaging in accordance with AP-17.1Q, *Record Source Responsibilities for Inclusionary Records*.

8. The investigator is responsible for security of the scientific notebook except after it is submitted to the Records Processing Center (RPC), given to the Responsible Manager, or to Reviewers, who then accept its security while in their possession.

9. Develop and maintain a table of contents on the initial pages set aside for this purpose (Paragraph 5.1.4) with the notebook entries that list the main topics or activities covered by the notebook, and applicable page numbers.

10. Laboratory, field, or log notebooks are not scientific notebooks unless they meet all requirements of this procedure. When used in support of a scientific notebook, these supporting laboratory, field, or log notebooks shall be referenced in a scientific notebook as a supplemental record and submitted as part of the scientific notebook records package.

Scientific Notebook Work Flow



The Control and Use of Scientific Notebooks for OCR/IMA Activities

CLASS004, Rev. 2

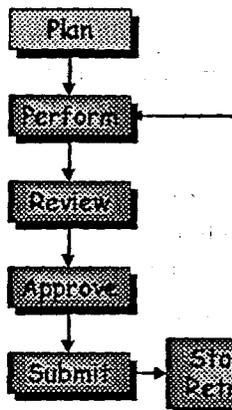
Notes

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Scientific Notebook Identification and Control

☞ Obtain a document identifier (DI) from the SN Register

☞ You will be prompted for the following:



- Organization

- Beginning date

- Title

- First & last name of responsible investigator

- Responsible manager

☞ Ensure SNs are organized and uniquely marked

☞ Document title, DI, and all interfacing notebooks in initial or final notebook entry

Notes

Obtain a document identifier for your scientific notebook through the Lotus Notes Scientific Notebook Register (SNR) database. Place the document identifier inside the front cover, on the first page, or on the notebook cover.

NOTE: Management control of the use, review, and closeout of scientific notebooks is maintained using a Lotus Notes database, the SNR. This database is a management tool to identify, track, and monitor the initiation and completion of the scientific notebooks. It can be added to your Lotus Notes Desktop using the Database Catalog.

NOTE: The identifier is made from a series of inputs as prompted, including the organization using the notebook. For example, a U.S. Geological Survey scientific notebook No. 2 would have the format SN-USGS-SCI-002, V1.

Organize notebooks as appropriate to the execution of the work and ensure that they are uniquely marked with notebook identifier, title and volume.

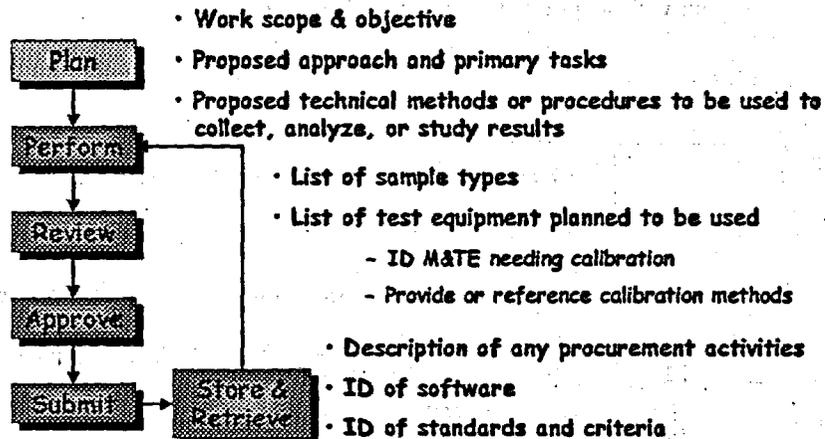
1) For a single notebook used on a given task, the SNR is programmed to provide sequential volume numbers for any identifier and title input.

2) For multiple related tasks, or task breakdown assignments, a "Master" notebook may be used that controls any series of supporting notebooks. Each volume shall be registered as in Step 1) above.

NOTE: For traceability of established notebooks, as applicable, title entries should begin with the original notebook identifier that may have been assigned by another organization's procedure or process.

Scientific Notebook Initial Entry

Record the following in the SN or reference an approved planning document:



Notes

Record an initial entry, in the scientific notebook, consistent with a work package or other planning document that includes or references the approved work package number, or other planning document that addresses the following planning information; then sign and date the entry:

- 1) The work scope including title of work, Work Breakdown Structure No., as applicable, research objective, proposed approach and primary tasks, or proposed technical methods or procedures to be used to collect, analyze, or study results.
- 2) A list of sample types giving details, as available and appropriate, for samples that are expected to be involved in the work activity.
- 3) A list of test equipment planned to be used with identification of measuring and test equipment needing calibration. Provide or reference the calibration methods and/or requirements including suggested calibration methods when appropriate, and indicate calibration schedule or frequency, if established.
- 4) Description of procurement activity pertinent to the investigation such as calibration or analytical services.
- 5) Identification of software to be used (include qualification status and Computer Software Configuration Item numbers).
- 6) Identification of standards and criteria, as applicable, including acceptance criteria.

Scientific Notebook Initial Entry (Cont.)

Record the following in the SN or reference an approved planning document:

Plan

- Any special training/qualification requirements
- Environmental conditions
- Potential sources of error

Perform

Review

Approve

Submit

Record the following in the SN:

- List of personnel expected to contribute to SN
- Include examples of signatures and initials
- ID responsible investigator
- ID any relevant information not included in referenced work planning documents or procedures

Store & Retrieve

Notes

7) Any special training/qualification including procedures, processes or skills; environmental conditions and accuracy precision or representativeness of results requirements (if different from the manufacturer's); and pertinent potential sources of error, as applicable.

NOTE: In lieu of the above information, the title and number of the applicable approved planning document(s), approved implementing documents, work instructions, or other documents containing this information may be referenced.

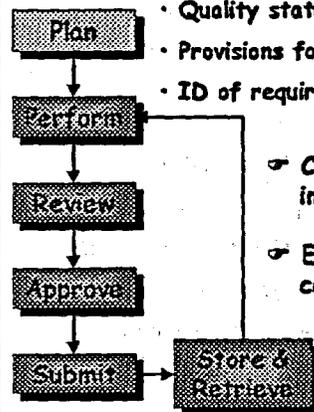
8) A list of personnel expected to contribute to the notebook, including examples of their signatures and initials. Leave reasonable space for modifications to this list. Identify the name of the investigator who is responsible for the notebook and its contents.

9) Additional relevant information that is not included in the referenced work planning documents, Implementing Procedures, or Technical Procedures, and any other information necessary to understand the research to be documented.

Scientific Notebook Initial Entry (Cont.)

☞ Record the following in the SN:

- Full citation of all work(s) referenced in SN
- Quality status of inputs
- Provisions for controls of any electronically managed data
- ID of required QA verifications, witness, or hold points



☞ Coordinate planning with organizations providing input to or using the results from SN

☞ Ensure initial entry is provided or referenced in concurrent volumes

☞ Initiate a compliance review of the initial entry (Attachment 2)

Notes

10) Full citation of all work(s) referenced in the notebook that is related to methodologies in the scientific investigation, and quality status, as appropriate.

11) Provisions for controls of any electronically managed data

12) Identification of any required QA verifications, witness, or hold points, etc.

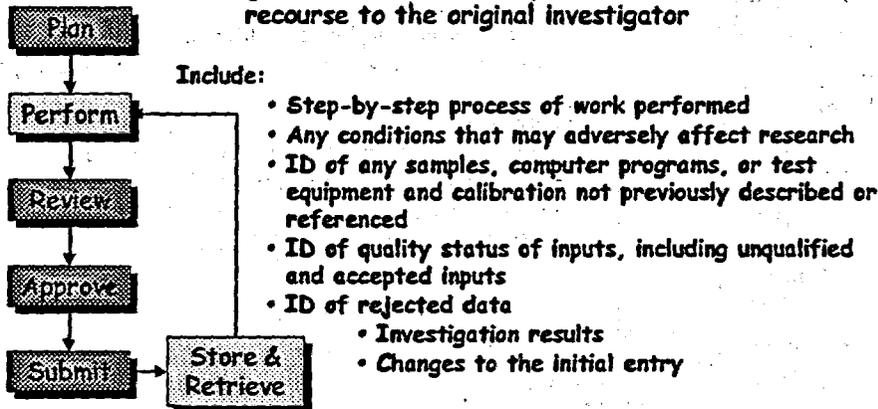
Coordinate planning with organizations providing input to or using the results from a scientific notebook. Provide the same initial entry information (or reference to an appropriate planning document, if applicable) in concurrent volumes of the scientific notebook or provide reference to the original initial entry at the beginning of each concurrent volume. All concurrent related volumes shall be cross referenced in their initial entries. Similarly, if applicable, provide an updated initial entry in effect at completion of a volume as a beginning to a new volume.

Initiate a compliance review of the initial entry using review criteria from Part 2 of the Scientific Notebook Compliance Review Worksheet (Attachment 2). Upon completion of the Initial Entry Compliance Review, evaluate the review and if acceptable, sign and date at the end of the initial entry. If unacceptable, return the scientific notebook to the Investigator with an explanation or further comments to be resolved.

Ensure that the investigator is aware of changes to any impacting planning documents and is directed to modify the initial entry as appropriate to maintain compatibility.

Scientific Notebook In-Process Entries

Document entries in sufficient detail to allow the investigation to be retraced and results confirmed, or repeat the investigation and achieve comparable results without recourse to the original investigator



Notes

Document the following in sufficient detail to allow a Technical Reviewer to retrace the investigation and confirm the results, or repeat the investigation and achieve comparable results without recourse to the original

Investigator:

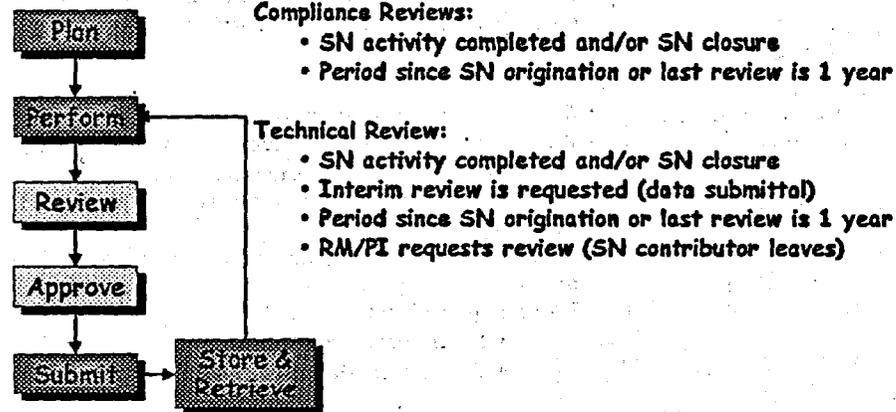
- 1) Step-by-step process of the work performed, including the accomplishment of prerequisite actions and any deviations from planned actions
- 2) Any conditions that may adversely affect the research described in each entry, if applicable
- 3) Identification of any samples, computer programs, or test equipment and calibrations not previously described or referenced, including quality status, as appropriate
- 4) Identification of any existing or accepted data that may be used in the investigation
- 5) Identification of any "rejected" and/or non-Q data, if known
- 6) Investigation results, including those that do not meet acceptance criteria
- 7) Interim conclusions, if any
- 8) Changes from or additions to the initial entry, including methods used, names, initials, and signatures of any new individuals performing the work. Include examples of initials and signatures.

Create a new notebook, but next higher volume, when all space in a notebook has been used.

- 1) Transfer updated initial entry that was in effect at completion of a volume, and use as a beginning to a new volume.
- 2) Refer to the new continuing notebook with a note at the end of the full notebook, to show it is being continued.

Scientific Notebook Review and Approval

Responsible Manager or PI (if not the investigator) initiates a compliance review, a technical review, or both



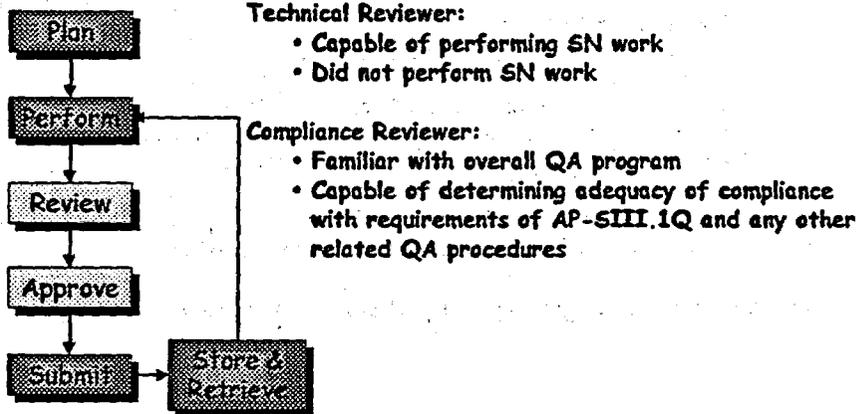
Notes

Initiate a Compliance Review or a Technical Review or both when:

- 1) The activity that is being documented in the scientific notebook has been completed, and/or the scientific notebook is being closed (Technical and Compliance Review)
- 2) An interim review is solicited by the Investigator, such as when the scientific notebook contains any data that may be used for analysis or submission to the Technical Data Management System (TDMS) (Technical Review)
- 3) The period since notebook origination or the previous review is approaching one year (Technical and Compliance Review)
- 4) The Responsible Manager/PI deems a review desirable, such as when a major notebook contributor leaves the work activity (Technical Review).

Scientific Notebook Review and Approval (Cont.)

Responsible Manager or PI (if not the investigator) selects a Technical Reviewer and/or a Compliance Reviewer



Notes

Select a Technical Reviewer who is capable of performing the described work, but who did not perform the work to be reviewed. Reasonable effort should be made to select a Technical Reviewer, who is not the Investigator's direct supervisor, when the notebook is being reviewed for closeout or submittal of any data to the TDMS (in accordance with Paragraph 5.6b).

Documented justification for the supervisor to perform the Technical Review shall be made directly or referenced in the scientific notebook.

- AND/OR -)

Select a Compliance Reviewer for scientific notebook compliance who is familiar with the overall QA program, and is capable of determining adequacy of compliance with requirements of this procedure and other related QA procedures listed in Section 7.0.

Evaluate and accept the Scientific Notebook Compliance Review following comment resolution by signing the "Review Approved by:" line in the header of the Compliance Review Checksheet.

Resolve the comments and document this resolution in the scientific notebook or, if the notebook is full, reference the documentation that will become part of the record package for the notebook.

Technical Reviewer



• Document review of SN:

- Information is technically adequate
- Information is presented in sufficient detail
- Software used is suitable to problem being solved
- Software used is within range of validation testing
- Detail concerns about technique, interpretation, or documentation
- Recommend further investigation, if appropriate

• Indicate SN has been reviewed and is technically adequate by making an entry in SN or other review documentation

• Include in entry beginning and end points of review

Notes

Perform a documented review of the scientific notebook using as a minimum the following criteria:

- 1) The information presented, including any referenced information, is technically adequate.
- 2) The information is presented in sufficient detail (including use of released software) to retrace the investigation and confirm the results or to repeat the investigation and achieve comparable results, without recourse to the original investigator.
- 3) Any software used is suitable to the problem being solved.
- 4) Any software used is within the range of validation testing.

Indicate that the scientific notebook has been reviewed and is technically adequate upon completion of comment resolution, by signing and dating an entry to that effect in the scientific notebook. This statement should be inclusive of supplemental records, include the beginning and end points of the review, and be at the end of the text and review comments for the reviewed material.

- OR -

Add comments or refer to other review documentation that detail concerns about technique, interpretation, and documentation, and sign and date the comments.

If appropriate, recommend further investigations by providing a statement to that effect in the scientific notebook, sign, and date.

Compliance Reviewer

- Document review of SN (use checklist or equivalent):
 - ☐ Provide justification for non-applicable criterion
 - ☐ Document non-compliance and provide explanation
 - ☐ Document compliance and provide comments as appropriate
- Return review documentation and SN to investigator for comment resolution
- Submit completed review documentation as supplementary record
- Reference review documentation in SN as close to end of SN segment reviewed



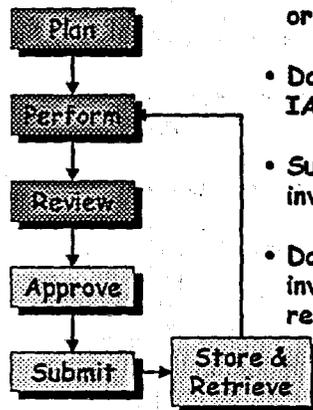
Notes

Review and document the compliance review by completing a form equivalent to that shown in Scientific Notebook Compliance Review Worksheet (Attachment 2).

- 1) Give justification of the nonapplicability of any criterion listed in the comment column.
- 2) Document any noncompliance by checking the "R" column as being reviewed, and making a comment concerning the deficient condition in the comments column.
- 3) Document compliance by checking the "R" column and provide supporting comments as appropriate to expand on the review results.
- 4) Return the review sheet and notebook to the investigator for comment resolution.
- 5) Initial each comment on the worksheet upon full resolution, and sign and date the review as being "Accepted," upon resolution of all comments.
- 6) Submit the completed review sheet as a supplementary record.

Reference the Compliance Review Sheet and any supporting documentation in the scientific notebook as close to the end of the scientific notebook segment reviewed as possible.

Data Submittal and Traceability



- Ensure relevant data used in analysis or that contributes to technical products or the collection of data is retrieved from the TDMS or TIC
- Document rationale for use of accepted data IAW AP-SIII.2Q
- Submit all data produced by the SN investigations to the TDMS IAW AP-SIII.3Q
- Data used as inputs to technical products involving scientific investigation shall be referenced in the SN using DTNs

Notes

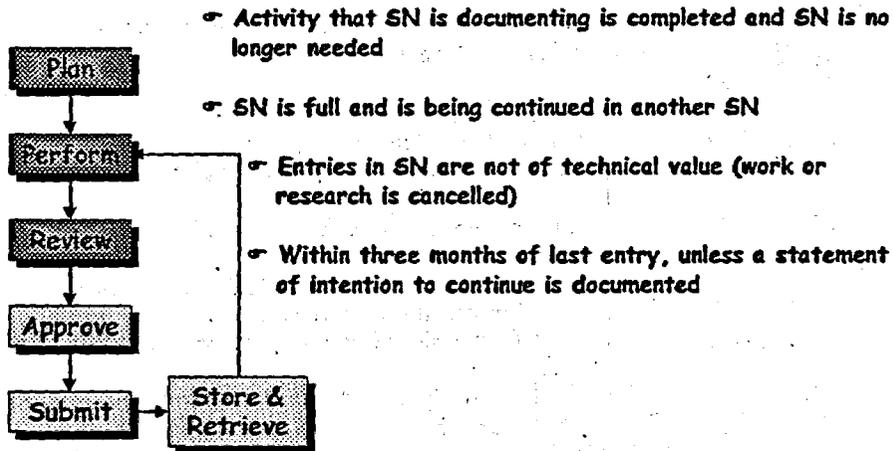
Ensure that any relevant data used in analysis or that contributes to technical products or the collection of data is retrieved from the TDMS or the Technical Information Center. If data retrieved from the Technical Information Center is to be considered accepted data, provide a rationale in accordance with AP-SIII.2Q, *Qualification of Unqualified Data and the Documentation of Rationale for Accepted Data*.

Submit all data produced by the scientific notebook investigations to the TDMS in accordance with AP-SIII.3Q, *Submittal and Incorporation of Data to the Technical Data Management System*, before any such data is used external to the scientific notebook investigation for analysis, etc., or otherwise prior to closure of the scientific notebook.

Data used as inputs to technical products involving scientific investigation shall be referenced in the scientific notebook using the TDMS Data Tracking Number (DTN).

Scientific Notebook Closure (Cont.)

Investigator closes-out the SN when:



Notes

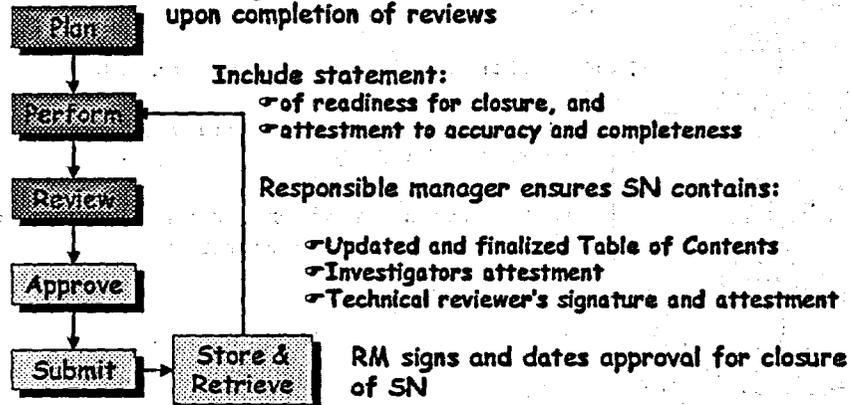
Close out the scientific notebook when:

- 1) The activity that the scientific notebook is documenting is completed and the scientific notebook is no longer needed
- 2) The notebook is full and is being continued in another notebook
- 3) It is determined that the entries in the scientific notebook are not of technical value; such as when work is cancelled for budget or reprogramming reasons, and the research being documented is discontinued
- 4) Within three months of the last entry, unless a statement of intention to continue with the notebook after a designated time is entered after the last technical entry.

Scientific Notebook Closure (Cont.)

Investigator requests a compliance and technical review

Investigator documents the closeout in a final entry upon completion of reviews



Notes

Request a Compliance and a Technical Review and document the closeout in a final entry upon completion.

Include a signed and dated statement of readiness for closure of the scientific notebook, and attesting to the accuracy and completeness of the information contained. When applicable, also include a Statement of Continuation in another volume. Place this final entry at the end of the notebook, and notify the Responsible Manager of this action.

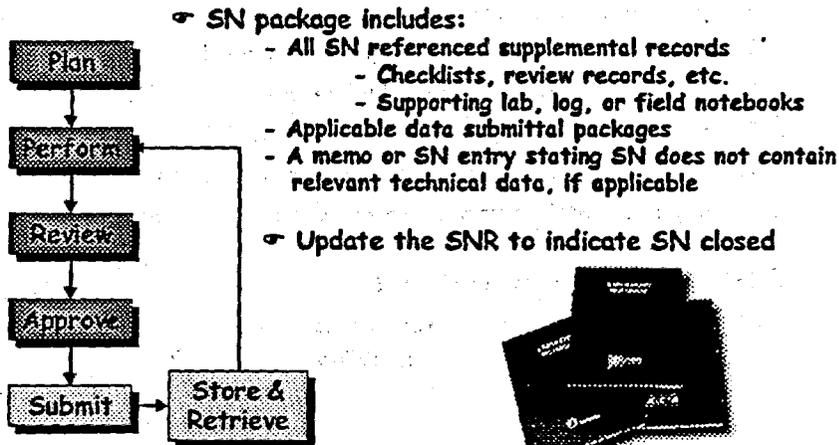
Ensure that the final scientific notebook entries include the following:

- 1) An updated and finalized Table of Contents.
- 2) Dated signature of the Investigator attesting that the information contained in the scientific notebook is legible, accurate, complete, appropriate to the work accomplished, in compliance with applicable procedures, and identifiable to the item(s) or activity(ies) to which the scientific notebook applies.
- 3) Dated signature of the Technical Reviewer stating that the scientific notebook meets review requirements and that all comments have been resolved.

Sign and date in the scientific notebook approval for closure of the scientific notebook and its submittal to the RPC; or return the scientific notebook to the owner for resolution of comments.

Records

Investigator submits SN to Records Processing Center (RPC)



Notes

Submit the closed scientific notebook to the RPC. The scientific notebook shall be accompanied by:

- 1) All scientific notebook referenced supplemental records.
- 2) Appropriate documentation to support Subsection 5.6, such as compiled data and the Data Tracking Number, in accordance with AP-SIII.3Q.
- 3) A memorandum signed by the PI, or the Investigator, or a copy of a signed entry at the end of the notebook, to the effect that the scientific notebook does not contain relevant technical data, if this is the case.

NOTE: It is encouraged to submit a copy of the notebook and its supplemental records, allowing the user to retain the original notebook.

Update the SNR database in Lotus Notes to indicate that the scientific notebook has been closed.

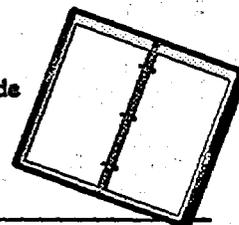
Records Package:

The closed out scientific notebook or segments of interim contributions to the scientific notebook, and if applicable, a memo signed by the PI or the Investigator indicating that the notebook does not contain relevant technical data.

The scientific notebook supplemental records, such as Technical or Compliance Review records, or supporting laboratory, field or log notebooks.

Typical Scientific Notebook Issues

- SN did not include enough details for independent, qualified person to determine work performed
- Initial entries in SN do not contain the required information
- SN not in accordance with procedure requirements and QARD
- SN pages not reviewed because SN not available
- Traceability of data and SN not consistently documented
- Planning of scientific investigation not performed in accordance with QARD
- Independent review not performed
- SN does not clearly identify references or provide adequate methodology for repeatability

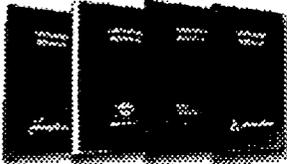


Notes

Lessons Learned and Suggestions for Improvement

Multiple notebooks, not cross referenced

Opinions/thought processes/logic trains difficult to follow - try to add more explanatory statements



Label sketches

Data and/or calculations in computer files, not referenced

Project jargon and cryptic notations - try to limit

Often, several notebooks were in use during one test and it was sometimes difficult to retrace the progress of the test. In cases like this, cross referencing between notebooks would be very helpful to later reviewers.

Opinions/thought processes/logic trains are the hardest thing to follow when trying to retrace the investigation without recourse to the original investigator. Try to add more explanatory statements. For example, rather than just stating air injection times were increased, state that "air injection times were increased because..."

Clearly label any sketches. A hand drawn sketch of a borehole video log looks remarkably like a hand drawn sketch of a length of core and a label eliminates any possible confusion. Similarly, label the axes of any sketched graphs.

Most of the notebooks examined were weak on stating testing requirements such as needed equipment or environmental conditions. More detail in these areas would be desirable.

Quite often data and/or calculations are in computer files, be sure to reference where and how to access these files in the scientific notebook.

Try to limit the use of project jargon and cryptic notations that require prior knowledge to understand. For example, a notebook entry that indicates, "the blue holes were tested" or "the red holes were tested" is not meaningful to a reviewer unless they have the color coded borehole layout from the Test Control Office (TCO) (and none of the notebooks examined included or referenced the color coded layout).

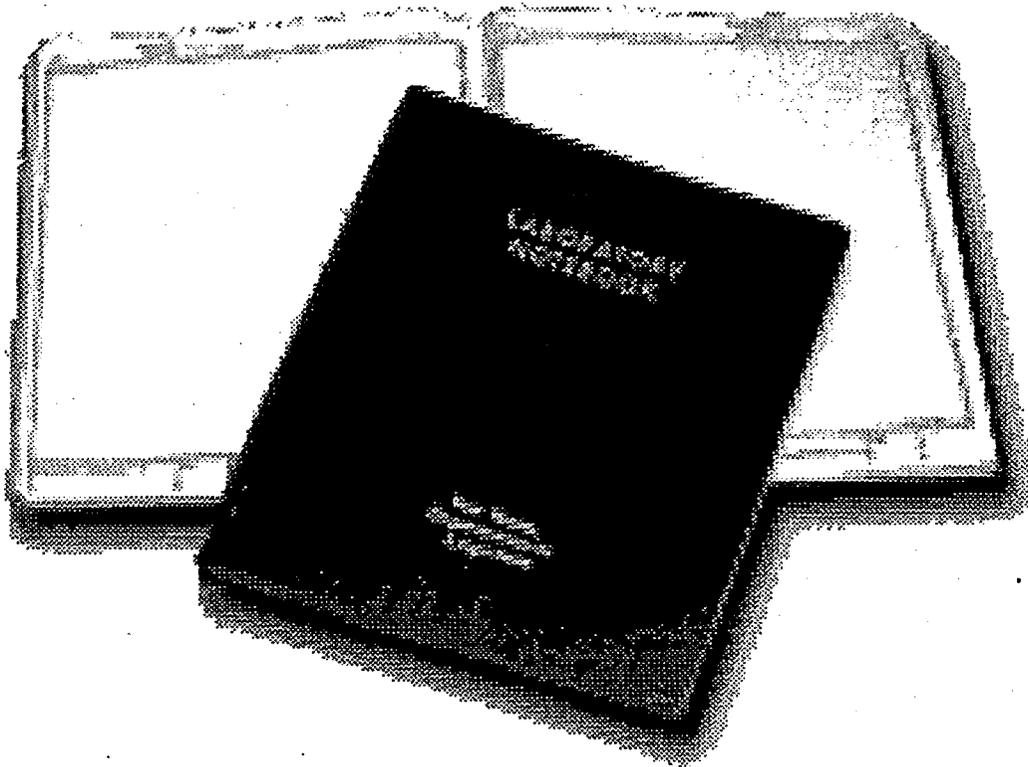
Summary

- What is the process for initiating a SN?
- What are the review requirements for a SN?
- What are the data submittal requirements?
- How is a SN closed-out and submitted?



Notes

***The Control and Use of
Scientific Notebooks for
OCRWM Activities***



***Scientific Notebook Compliance Review
Worksheet***

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT SCIENTIFIC NOTEBOOK COMPLIANCE REVIEW WORKSHEET			
SN:		Local ID:	Investigator:
Title:			
Reviewed By:	Reviewer Organization:	Date:	
Review Accepted By:	Acceptance Date:	Record Submittal Date:	
Applicable Implementing Document (Include Rev. No.):			
Requirements/Criteria	R	NA	Comments (See Note)
1. Notebook Initiation Includes:			
a. Unique Identifier and Start Date			
b. Use of Bound Book			
c. Space for Table of Contents			
d. Continuous Pagination			
e. Reference any Preceding Notebook			
f. Legible and Reproducible			
2. Initial Entry Includes Following: (for a Referenced Planning Document)			
a. Objective and Description of Work			
b. ID of Scientific Approach or Technical Methods Used to Collect, Analyze, or Study Results			
c. ID of Applicable Standards and Criteria			
d. Equipment to be Used			
e. ID of M&TE and Calibration Requirements			
f. Special Training/Qualification Requirements			
g. ID of Prerequisites, Special Controls, Environmental Conditions, Processes or Skills			
h. Accuracy, Precision, and Representativeness of Results			
i. Identification of Software			
j. Identification of Samples			
k. List of Related Procedures to be Used			
l. ID of QA Program Verifications			
m. List of All SN Users/Signature/Initials			
n. Designated Owner of SN			
o. Planning Coordinated with Organizations Providing Input to or Using the Results			

EXAMPLE

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT SCIENTIFIC NOTEBOOK COMPLIANCE REVIEW WORKSHEET			
SN:			QA: Page: 2 Of: 2
Requirements/Criteria	R	NA	Comments (See Note)
3. In Process Entries Include:			
a. Description of Work Performed and Results Obtained			
b. Compliance with OAFD Supplement V			
c. Compliance with Modeling Documentation			
d. Changes/Additions to Initial Entry Information			
e. ID of any Unqualified (Existing) Data Used			
f. Trace to Attachments/Related SNs			
g. Names Who Performed Work			
h. Signature/Date of Each SN Entry			
i. Description of Changes to Methods Used			
j. Interim Conclusions as Applicable			
k. Explanatory Statement When Dormant			
4. Notebook Review Includes:			
a. Initial Entry Review			
b. Technical Review (Paragraph 5.5.4)			
c. Compliance Review (Paragraph 5.5.3)			
d. Any Referenced Material Needing Review			
e. Adversely Affecting Conditions			
f. All Comments Resolved			
5. Notebook Closeout Includes:			Completed Only After Notebook Has Been Closed Out
a. Independent Technical Review of Notebook			
b. Compliance Review of Notebook			
c. Statement of Acceptability by Manager			
d. Data Was Submitted to TDMS			
e. Records Check			
f. Records Package Was Submitted			

EXAMPLE

Note: Legend: R - Review accomplished in accordance with this criterion; NA - This criterion is not applicable to this notebook; Comments - Explanation of non-compliance issues, explanatory notes or justification of non-applicability, as applicable.

The Control and Use of Scientific Notebooks for OCRWM Activities



Work Plan Example



**TRW Environmental
Safety Systems Inc.**

**1180 Town Center Drive
Las Vegas, NV 89134
702.295.5400**

**WBS: 1.2.3
QA: L**

MOL.19980217.02

**Contract #: DE-AC01-91RW00134
LV.NEPO.ATRS.NEB.1/98-011**

January 29, 1998

To: Distribution

Subject: Work Plan for Integrated Site Model

In accordance with procedure QAP-SIII-1, work plans are to be developed for planned scientific investigations. These work plans are to be reviewed by the effected organizations, users of the results of the investigations, and Quality Assurance. Attachment 1 is Rev. 0 of the work plan developed for the Integrated Site Model (ISM) effort, of which the following organizations are a user through either the incorporation of the ISM stratigraphy and properties into repository design models (for EBSO), process models (for NEPO), or performance assessment models and the Technical Data Base (for PAO). Accordingly, we are requesting a review from the persons listed below for these affected organizations. The focus of the review is the assessment of whether the document fulfills the requirements of a work plan, as specified in Section 5.1.2.B of procedure QAP-SIII-1, and particularly in light of the needs of the reviewer's organization. This section of the procedure is included as Attachment 2. If a reviewer has comments on the plan, he/she is requested to provide the comments to Norma Biggar in either a memo, by e-mail, or as comments in the margin of the plan, as specified in review guidance in QAP-SIII-2. Mandatory comments are to be indicated accordingly. Concurrence with the work plan is to be indicated by signature on the form in Attachment 3 (after QAP-SIII-2).

**Engineered Barrier System Operations (EBSO): Robert Elayer
Natural Environmental Program Operations (NEPO): Dwight
Hoxie
Performance Assessment Operations (PAO): Steve Bodnar
Office of Quality Assurance (OQA): Catherine Hampton**

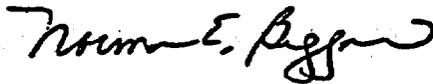
LV.NEPO.ATRS.NEB.1/98-011

January 29, 1998

Page 2

If you have any questions or comments please contact Norma E. Biggar at 5-3549.

Sincerely,



Norma E. Biggar, Technical Lead, Geology
Natural Environment Program Operations
Management and Operating Contractor

NEB/kb

Attachments:

- (1) Work Plan for ISM
- (2) Section 5.1.2.B of Procedure QAP-SIII-2
- (3) Reviewer's Statement and Responsible Manager's Approval

Distribution:

C. E. Hampton, DOE/YMSCO, Las Vegas, NV, MS 523
L. R. Hayes, M&O, Las Vegas, NV, MS 423/1265
R. D. Snell, M&O, Las Vegas, NV, MS 423/1259
J. L. Younker, M&O, Las Vegas, NV, MS 423/1259

cc:

LVRPC=8

Work Plan for Integrated Site Model**Revision 0****December 23, 1997****1.0 Work Scope**

This work plan is applicable to Integrated Site Model (ISM) work that is conducted under the M&O quality assurance procedures. This work encompasses all phases of model development, including data compilation, data analysis, model construction, model analysis, and preparation of model products. Supervision of a Numerical Model Warehouse (NMW) and translation of model components between software formats are also included. The work scope is as defined during the annual planning process, and documented in project-approved annual planning documents and Participant Planning Sheets (PPS) for a given fiscal year.

1.1 Objective

The objectives of the Integrated Site Model (ISM) work are to provide the YMP with reference geologic framework and integrated rock properties models on which flow, transport, and performance assessment studies will be based; and to serve as a repository for preliminary 3D models and model components.

1.2 Primary Tasks

Primary tasks of the ISM work include:

- 1) **Compilation and analysis of input geological data, including detailed reviews of potential model input data provided by others;**
- 2) **Construction of a three-dimensional geologic model of rock units and faults at Yucca Mountain;**
- 3) **Incorporation of 3D rock properties and mineralogic models into the geologic framework model;**
- 4) **Creation of model products (maps, cross sections, views, animations, illustrations)**
- 5) **Preparation of reports of model results;**
- 6) **Serve as "gatekeeper" for the Numerical Model Warehouse of the Technical Data Management System, which houses electronic files of 3D models, input data, and model products for use by Yucca Mountain Project (YMP) modelers;**
- 7) **Translation of model components between software formats**

1.3 Use of Data

Input data will be compiled from existing YMP documents in the Records and Technical Database systems. No new data will be acquired under the scope of this work; however, data may be reinterpreted during the iterative process of model development. Data qualification

status and reference document of each input data point will be maintained and recorded. Interpretations and their technical bases will be documented.

2.0 Methods and Approach

The geologic framework model will be constructed using standard procedures for the Earthvision 3D modeling software, outlined as follows. The process and interpretations made by the modeler(s) are documented in a Scientific Notebook (procedure QAP-SIII.3Q) as appropriate, one notebook for each model version. Input geologic data will include borehole lithostratigraphy, geologic maps, measured sections, and tunnel lithostratigraphy, and will be used to construct grids for faults, reference horizons, and isochores. Geophysical inputs include interpretations of gravity, magnetic, and seismic data. Grids will honor input data. Each grid will be controlled by the modeler to represent a reasonable geologic interpretation for that feature, i.e., the software will not be given free rein to construct surfaces based solely on mathematics. The modeler will control the assembly of faults and horizons into the geologically correct sequences and with the correct geometric and geologic relations by definition of input parameters. Each step of the modeling process will be iterated until the desired results are achieved; that is, until the modeled feature represents the modeler's interpretation of that feature and honors the input data.

A minimum number of reference horizons will be constructed, from which the thicknesses of the remaining units will be added or subtracted. The number of reference horizons will be minimized to reduce model construction time and reduce potential user-induced grid errors such as overlaps or gaps between successive units. The number and identity of reference horizons will be determined by iterative construction of interim models. Each iteration will be analyzed for correct fault offsets, correct horizon extrapolation, intercept with input data points, and intended horizon configuration. Grids or parameters will be corrected as needed. When the geologic framework has been completed for a model version, this will be documented in the scientific notebook for that version.

The 3D rock properties and mineralogy models (and others as appropriate) are generated under other activities outside of this work scope, and will be received in a format readable by Earthvision software. This format generally consists of grid nodes with regular horizontal spacing and regular or variable vertical spacing. Each grid node contains x and y coordinates, z elevation, and a property value. These grid nodes will be input to the geologic framework model as grid nodes, and will not be manipulated or extrapolated. If required, grid nodes will be shifted to exactly match the top and bottom horizons which bound the modeled rock body. The modeling software is then used to construct 3D contours around the grid nodes to visually represent the rock properties or mineralogic model. This constitutes integration of the rock properties models into the geologic framework to construct the integrated site model (ISM). When the ISM iteration is considered complete, this will be documented in the scientific notebook.

The ISM workscope also includes serving as the "gatekeeper" to the The Numerical Model Warehouse, which is an on-line, computer-based storage facility for 3D model components and products for use by YMP modelers. The Warehouse is maintained and managed by the Technical

Data Management System as part of the YMP GENISES technical data base, and will physically reside along side GENISES. The ISM modelers will maintain a separate computer facility for the exchange of preliminary and interim models and data, and to serve as the receiver of models to be submitted to the NMW. The ISM work scope includes the translations between modeling formats, and the selection of models to be submitted into the NMW formats. This process is also documented by scientific notebook.

Software tools to translate model components will be constructed both by the ISM modelers (for simple cases) and by outside contractors (for complex cases). All translations will be performed by the ISM modelers. The translation tools are not required to be qualified under QARD requirements because the translation algorithms simply reproduce the model components in a new format (comparable to translating between word processing document formats), they do not perform mathematical manipulations of data, and they do not produce new data or interpretations. Translations will be validated by comparison of outputs of the original model versus the translated version.

3.0 Applicable Standards and Criteria

No applicable standards and criteria have been identified as applicable to the ISM effort.

4.0 Developed Procedures and Implementing Documents

Implementing documents specific to the modeling work will include M&O QA procedures QAP-SI-0Q (computer software qualification), QAP-SIII-1Q (scientific investigation control), AP-17.1Q (name##), QAP-SIII-2Q (review of scientific documents and data), and QAP-SIII-3Q (scientific notebooks).

5.0 Equipment

No testing, field, or laboratory equipment will be used. Computers will be used for modeling.

6.0 Records and Reports

This work will be recorded in Scientific Notebooks by each involved investigator in accordance with M&O QA procedure QAP-SIII-3Q. Reports will be developed as required in deliverable criteria as established in the annual planning process, and in accordance with M&O QA procedure QAP-SIII-1Q. Records will be submitted in accordance with M&O QA procedure AP-17.1Q.

7.0 Prerequisites, Special Controls, Environmental Conditions, Processes

No applicable prerequisites, special controls, environmental conditions, or processes have been identified as applicable to the ISM effort.

8.0 Computer Software

The 3D geologic modeling will be conducted using Earthvision software manufactured by Dynamic Graphics, Inc., of Alameda, California, on Silicon Graphics computers running the IRIX operating system. The current, Qualified software version will be used on hardware specified in the currently applicable Software Qualification Report (SQR). The Earthvision version 3.1 Computer Software Configuration Identifier (CSCI) number is 30008 v3.1, and the SQR accession number is MOL.19970115.0226. Software revisions or updates used in developing ISM components will be qualified in accordance with M&O QA procedure QAP-SI-00. The concept of "validation range" does not apply to geologic framework modeling software.

9.0 Evaluation of Results

The geologic framework model will be validated by comparison of outputs to input data values. The model will be deemed satisfactory if final model values for elevation are within 3 feet of input elevations at boreholes. This number was determined by sensitivity analysis of the effects of elevation on rock properties model results, and represents the value at which adverse effects appear in properties models. This number does not reflect the model's predictive capabilities or imply accuracy of the input data, but is strictly a comparison of model inputs and outputs.

The geologic framework model will also be evaluated as new boreholes are completed by comparing lithostratigraphic elevations in the borehole with those predicted by the model. The sources of error will be evaluated and the model revised accordingly.

10.0 Interfaces Across M&O Areas

Potential geologic data inputs will be received from the U.S. Geological Survey, and will be reviewed and analyzed as part of the iterative modeling process. The geologic framework model will be translated to software formats compatible with other 3D modeling software packages used in the YMP, and the results transmitted electronically. Model version number will be explicit in each electronic file name, and text will accompany the transfer to provide reference documents and data traceability. Customers for the geologic framework model include the M&O Mined Geologic Disposal System (MGDS) Design, Performance Assessment, and Scientific Programs Office (SPO) groups, including the unsaturated zone flow model, the saturated zone flow model, the radionuclide transport models, and the repository design model. In addition, products will be developed from the geologic framework model to be used for SPO and DOE management purposes, including maps, cross sections, views, and calculations.

ATTACHMENT 2

Section 5.1.2.B of Procedure QAP-SIII.2

- B.** if no previously approved work planning document exists, prepare a document that provides the following information, as appropriate:
- 1.** definition of the work scope, objectives, and a list of the primary tasks involved;
 - 2.** identification of the scientific approach or technical methods used to collect, analyze, or study results of applicable work;
 - 3.** identification of applicable standards and criteria;
 - 4.** identification or development of appropriate procedures or other implementing documents;
 - 5.** identification of field and laboratory testing equipment or other equipment;
 - 6.** identification of, or provisions for the identification of, required records and report preparation (e.g., scientific notebooks and scientific documents);
 - 7.** identification of prerequisites, special controls, environmental conditions, or processes;
 - 8.** identification of any computer software to be used that is subject to QARD requirements, by computer type, program name, version/revision number, Computer Software Configuration Item number, and validation range;
 - 9.** provisions for determining the accuracy, precision, and representativeness of results; and
 - 10.** identification of any interfaces and interface controls that transcend boundaries between M&O areas including quality assurance (QA) verifications of the work to be performed; then
- C.** provide the work planning document to the Responsible Manager.

ATTACHMENT 3

**REVIEWER'S STATEMENT AND
RESPONSIBLE MANAGER'S APPROVAL**

As a Reviewer for the _____ organization, I have reviewed Rev. 0 of the Work Plan for Integrated Site Model, in accordance with the content criteria specified in QAP-SIII-1/Rev. 2, Section 5.1.2.B. I verify that the document meets review requirements and all of my mandatory comments have been resolved. (If this is not the case, so state and attach the mandatory comments that were resolved by management.)

Signature

Date

Organization

As the Responsible Manager for the above document, I certify that a review has been conducted and that the document is ready for further action in accordance with Section 5.1.3 of QAP-SIII-1.

Signature

Date

Organization

***The Control and Use of
Scientific Notebooks for
OCRWM Activities***



Scientific Notebook Example

Scientific Notebook Compliance Review Worksheet

RL-Cof

SN-M&O-SCI-003, V1; Local ID Same ;

Owner: Robert Clayton

MOL. 19990521.020

Title: Integrated Site Model (ISM) Version 3.0

Organization: M&O/NEPO

Reviewed By: Darrell Porter ;

Organization: M&O/NEPO; Date 03/30/99

Review Accepted By _____

Date / / Record Submitted / /

Applicable Implementing Document (Incl Rev No.): OAP-SIII-3, R2

Requirements/Criteria	R	NA	Comments: (See Note 4)
1. Notebook Initiation Includes:			
a. Unique Identifier and Start Date	X		Ok
b. Use of Bound Book	X		Ok
c. Space for Table of Contents	X		Ok
d. Continuous Pagination	X		Ok
e. Reference any Preceding Notebook	X		Ok
f. Legible and Reproducible	X		Ok
2. Initial Entry Includes Following: (or a Referenced Planning Document?)			
a. Objective and Description of Work	X		OK
b. ID of Scientific Approach or Technical Methods Used to Collect, Analyze, or Study Results	X		Ok
c. ID of Applicable Standards and Criteria	X		Ok
d. Equipment to Be Used	X		Ok
e. ID of M&TE and Calibration Requirements	X		Ok
f. Special Training/Qualification Requirements		NA	OK; No special training is required
g. ID of Prerequisites, Special Controls, Environmental Conditions, Processes or Skills		NA	OK: There are no prerequisites, special controls, environmental conditions processes or skills involved
h. Accuracy, Precision, and Representativeness of Results	X		Ok
i. Identification of Software		NA	OK; Considerable software involved but inadequate description in the initial entry and qualification needs for it.
j. Identification of Samples	X		Ok. No samples involved
k. List of Related Procedures to Be Used	X		Ok
l. ID of QA Program Verifications	X		Ok. They are subject to annual audit
m. ID of Required Records	X		OK
n. List of All SN Users/Signature/Initials	X		Ok
o. Designated Owner of SN	X		Ok
p. Planning Coordinated with Organizations Providing Input to or Using the Results	X		Ok

Requirements/Criteria (Cont)	R	NA	Comments (M&O-SCI-003 Cont)	Page 2 of
3. In process Entries Include:				
a. Description of Work Performed and Results Obtained	X		OK	
b. Compliance with QARD Supplement V		NA	OK: No data in this notebook is managed electronically	
c. Compliance with Modelling Documentation	X		OK	
d. Changes/Additions to Initial Entry Information	X		Ok	
e. Id of Any Unqualified (Existing) Data Used.	X		Ok	
f. Trace to Attachments/Related SNS	X		Ok	
g. Names who Performed Work	X		Ok	
h. Signature/date of Each SN Entry	X		Ok	
i. Description of Changes to Methods Used	X		Ok	
j. Interim Conclusions as Applicable	X		Ok	
k. Explanatory Statement When Dormant	X		Ok	
4. Notebook Review, Includes				
a. Initial Entry Review	X		Ok: Initial review is not used as a planning document	
b. Technical Review	X		Reviewed by McCleary on 03/17/99	
c. Compliance Review	X		Ok: Markers for Inconsequential corrections were made	
d. Any Referenced Material Needing Review	X		Ok	
e. Adversely Affecting Conditions	X		Ok	
f. All Comments Resolved	X		Comments on 4.b must be resolved	
5. Notebook Closeout Includes:			Completed Only After Notebook Has Been Closed Out	
a. Independent Technical Review of Notebook		NA	Notebook has not been closed out.	
b. Compliance Review of Notebook		NA	" " " " "	
c. Statement of Acceptability by Manager		NA	" " " " "	
d. Data Was Submitted to TDMS		NA	" " " " "	
e. Records Check		NA	" " " " "	
f. Records Package Was Submitted		NA	" " " " "	

Note 1 Technical Review: a) Ability to retrace investigations and confirm the results or b) repeat the investigation and achieve comparable results, both without recourse to the original investigator. [snrctcklist_1]

Note 2 Compliance Review: A review of applicability, correctness, technical adequacy, completeness, accuracy, and compliance to established requirements.

Note 3 Records Check : Determines if record is legible, accurate, complete, appropriate to work accomplished, and identifiable to active case.

Note 4 Legend: R for reviewed; NA for not applicable; Comments for explanation of compliance issue, or justification of non-applicable.

Scientific Notebook Register

Scientific Notebook ID SN-M&O-SCI-003-V1

Date Opened 02/02/98

Notebook Title INTEGRATED SITE MODEL (ISM) VERSION 3.0

Last Name CLAYTON First Name ROBERT

Responsible Manager NORMA BIGGAR

WBS Number (Optional) 1.2.3.9.5

Mead

SCIENTIFIC NOTEBOOK

Integrated Site Model
(ISM) Version 3.0

SN-1120-SC1003-V1

Robert W. Clayton

70 SHEETS
COLLEGE RULED
11 x 8½ in / 27.9 x 21.5 cm
1 SUBJECT NOTEBOOK



Scientific Notebook for ISM3.0

Robert W. Clayton

Feb 2 1998 RLWC

This notebook is being conducted in accordance with CRWMS M+O Quality Assurance (QA) procedure ST-E-3 Rev.2.

This work is being conducted in accordance with "Work Plan for Integrated Site Model"

The objectives of this activity are:

- 1) Construct a geologic framework model from updated data sources, specifically the USGS re-evaluation of brechele lithostratigraphy by R.W. Spangler and D.C. Juresch. Use as a starting point previous 3D models and other YMP literature. Input data evaluation and editing are important phases of this activity.
- 2) Incorporate rock properties and mineralogy models into the geologic framework model (GFM) to construct the Integrated Site Model (ISM). Assist in translation of data, models, and model components as required.

SOFTWARE: Earthvision version 4.0

CSCI 30035 V4.0 DI 30035-2003 V4.0

MI 30035-M09-001

HARDWARE: Silicon Graphics Octane with 2, R10000 processors,
Operating System ^{Rev 1/20/98} IRIX 6.4.

Notebook Entries: Robert W. Clayton signature: RLWC
initials = RLWC

Parallel Notebooks: Robert Elayer
Jennifer Hinds

(Feb 2 1998 cont'd) PLWFC

I will mark on only ONE side of each page. Pages are numbered sequentially.

EXPECTED RESULTS: I anticipate finding a small number of errors or inconsistencies in the input geologic data. The charter of this model is to use only the best available technical data; therefore, if a data value can not be verified and appears to be anomalous, it will not be used and a justification will be written.

Each component of a model is INTERPRETIVE and is constructed based on the P.I.'s professional judgement. At times these judgements are tempered by other interpretations or by specific technical or logistical needs. For example, design of a parking tunnel may require that only the most technically sound input data be used and that the relevant interpretations be the most sound and justifiable.

The model is expected, or anticipated to be so in the repository area, while more interpretive latitude may be used in outlying areas where data are sparse.

More on these topics in following pages.

Accuracy + Precision +

SOURCES OF ERROR: Barely input data have been rigorously reviewed, but some typographical errors could conceivably come through.

Some "error" or mismatch of final surfaces to input data could be caused ^{PLWFC 1/20/98} by modeling-related necessities, like replacing zero's in inchare grids with slightly negative numbers to avoid coplanar surfaces and produce better pinchart edges.

The software itself is anticipated to have each datum

(Feb 2 1998 cont'd) JLR-C

to within about 0.25 feet on appearance and testing
have shown.

LIMITATIONS: First, a model is only an interpretation.

Second, we can not model every fault or every

rock layer due to time, data, and software/hardware

limits. Third, the model is a big and complex

task. Some details are likely to slip through.

Fourth, we have only 4 weeks to complete what used

to have been (and should be) a 16-week job

To overcome this, I will be working overtime (and won't

get paid for it - but that's another issue).

Fifth, 6160 implies "garbage in, garbage out." The

model can not represent the quality of the information

beyond the quality and consistency of the data.

Training & Qualifications: Now beyond my written description on file.

But in general this modeling requires training on the software

and geologic education & background involving volcanic rocks.

I have trained at Dynamic Graphics on the entire software

package. My M.S. thesis was modeling & analyzing faults in

each of the three fault lines at Yucca Mtn, and I have a Ph.D.

in Geological Science. I have been creating 3D models

of geology for 10 years.

Geologic Framework Model: A collection of digital files comprising a

geologic interpretation of a volume.

Superseded model versions are deleted, but only after the

new version is carefully evaluated and determined to be better.

This page reserved for additional notes

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2/16/99 RUES APPENDIX:

The Qualification status of all data used in both GEM and ISM 3.0 will be documented in the ISM report. The data are too numerous and bulky to be included here. All

GEM data reside in the TDMS system. Efforts are underway to ensure that all properties and min/pet data are also

submitted to TDMS — in some cases, the H's have been in possession of the data since before TDMS was initiated. The Q status

and submittal of data are beyond my direct control, but I have made the appropriate requests to have them qualified. ^{see 2/16/99} ~~to GEM~~

In general as of today, borehole data are non-Q/TBV; geologic map is Q/TBV; post-1991 measured section are Q/TBV; pre-1991 measured section are non-Q. The TBV means Q other times are being worked. We fully expect nearly all borehole data to become Q.

Table of Contents

Initial Entry	i
Table of Contents	v
Begin	1
File Naming Convention	2
Notes on Scheduling	5
End	22
Manager's Review	23
PART II: Integration of Rock Property & Mineralogic Models	24
End of notebook	28

2/12/98 PLP-EC

ISOCHORES

Meeting on EA approval of Earthworm's Software Qualification Report. So for the time being, I'll only use methods that are most mirrored in the qualification - drawing, mapping, and display. Will use EY 3.1 (6) for guidance at this stage. I am in charge of conducting the isochore maps for the pre-Topogal units. Joel Elyas does the Topogal, and Demetris Havel does the post-Topogal units. I also do alluvium and the structural reference horizon at base of Tera (top of bT4).

The attachment on the next couple of pages shows the naming convention for ISM3.0 files.

Here's the process of use to construct isochores:

- 1) Plot out map, the new data to see how it looks.
- 2) Create a file for any interpretive contours. This file name has "RUC" in it.
- 3) Show as few interpretive contours as needed to make the map look like I want. In Earthworm's, this means a relatively even distribution across the map.
- 4) Keep this up until the map is satisfactory.

DEFINITION: ISOCHORE means vertical thickness. In contrast, isochor means stratigraphic thickness, where effects of age are removed.

PHILOSOPHY: My interpretive philosophy is to create a generic map that shows all data and strives to be an accurate qualitative tool as opposed to making an interpretive statement.

intentionally left blank

Attachment : ISM3.0 File Naming Conventions

General

The following guidelines may help us keep straight the many files we will create for ISM3.0. Files will be named in the following general format:

[id][3][name][version].[suffix]

where id=source or type identifier 3=ISM3.0 name=rock unit or fault name version=version of data or model and suffix=file type.

The *id* field will consist of the following:

- a=all relevant data; combined sources
- b=borehole-derived
- e=ESF-derived
- f=fault
- i=isochore
- m=geologic map contacts or traces
- x=measured section
- p=property
- s=surface; elevation

Version can also be X=transposed ED=edited OLD=superseded RWC=Robb Clayton's edits EXP=exported file, etc. These will be the ONLY CAPITALIZED letters in file names.

<suffix>=file type; .txt for ASCII text, .dat for Earthvision data, .xls for Excel spreadsheet, .lyn translated files, and so forth.

Examples:

b3tpmn00.dat

is a data file with borehole data for unit tpmn, version 00.

s3tpv389.2grd

is a 2D grid file of a surface (elevation) for unit tpv3, version 89.

id fields can be combined where appropriate:

sm3pbt402.dat

is a surface (elevation) data file with map-derived contacts for Paintbrush Group bedded tuff 4, 02. In a combined *id* field like this, the *i* or *s* will always come first. The file:

sa3pbt412.dat

would be a surface data file for bedded tuff 4 with all data sources combined (map, borehole, etc.)

Where items are self-explanatory, the full names will be used. Examples include topography.2, potentiometric.dat.

Input Data

(Naming Conventions cont'd)

3

The finalized borehole contacts will be *borestrat98.dat*. The location data of newly surveyed borehole collars will be *boreholes98.dat*. Earthvision format files for display of holes as tubes will be *boretubes98.dat*. ESF contacts will be in *esfstrat98.dat*.

Stratigraphy

All rock layers will be referred to by their officially approved lithostratigraphic name and abbreviation from Buesch and others OFR 94-469 and Sawyer and others GSA Bulletin 1994.

Rock layer names will be spelled out in full in file names, beginning with formation. For example, rock layer Tptpmn will be named "tpmn". Calico Hills formation will be "ac". Bedded tuffs will take the name of the overlying units. For example:

i3pbt2RWE03.dat

is an isochore data file for the Calico Hills formation edited by Bob Elayer, version 03.

Faults

Where named on a geologic map, a fault will be given the map name. Otherwise, a simple name will be given that relates the fault to a named fault or a geographic feature. For example:

fm3dunew200.dat

contains map fault trace data ("fm") for a fault named "dunew2", version 00. This fault is the second strand west of the fault called "dune" on the maps (the Dune Wash fault).

Earthvision Files

Because these files are uniquely identified by their suffixes, no "id" field is needed.

.seq: Sequence files fall into three categories: pre-horizon gridding, post-horizon gridding, and spec. The post-horizon gridding sequence file names the horizon grids in each fault block, while these are in the pre-horizon gridding file. It is often important to separate the two and maintain them for further modification. Use of "pre" and "post" is a simple way to identify these files. For example:

3pre00.seq

will be the first sequence file constructed. It will be followed by 3post00.seq. Other sequence files for building test cases or submodels can be given similar short, descriptive names.

.faces: The first .faces file built will most likely be 3all00.faces, containing all horizons. Submodel could include 3paint00.faces (Paintbrush Group units only), or 3crater00.faces (Crater Flat Group or

Formulas, Scripts, Graphics, etc.

These files should be given descriptive names that will be easily identifiable long after we've forgotten them.

2/3/98 RLVSC

[SCHOERS] cont'd

Continued work on the me-topogms sketches and got them to where I want them. I think the sketches might give produced achieve what I stated in my continuing philosophy statement on page 1.

INPUT DATA NOTES: For the Coates Flat (Glynn area) (Row, Bullock, Tramm) the 1855 has given me non-depositional units. The vitric crystalline and welding units are not necessarily stratiform; therefore, each vitric may not necessarily make sense as a depositional/formed unit as geologists are accustomed to thinking. They instead reflect post-eruption processes that are not necessarily parallel to depositional stratigraphy. The top units of each Tuff are also variably eroded, so on the maps you'll see local base.

Interestingly, many of these units show a strong thickness difference between the "c" holes and pit 1. Most units are thinner at pit 1, but a couple are thicker. One given these includes a gentle trend to infer that pit 1 was on top of a persistent high block (which I think was the Raintown fault system).

INPUT DATA NOTES: I would have correlated the logs (density log, primarily) differently. I believe I can see collective units that differ from the v-c units and are more clearly depositional. But it was decided that the v-c units are the divisions needed by flow and transport models, so that's what we're using.

GENERAL FLAT UNITS:

where RLVSC 2/3/98

- PROWV - upper crystalline
- PROWC - upper crystalline
- PROWD - moderately to densely welded
- PROVSC - lower crystalline
- PROVSV - lower vitric

} battle names for Bullock (bull) and Tramm

2/4/98 RWC

Base TNA Structural Reference

I'm modifying the surface used in GFM2.1, updated with new borehole data from the USGS.

Chris Potter and Bob Dickerson (USGS Structures) provided extensive comments to me about cross sections through GFM2.1. I'm working on incorporating these comments, which mostly concern fault effects and stratal dips.

Again with this surface (as with isobars), my philosophy is to keep it simple and let the data speak.

INPUT DATA for this surface are borehole contacts and the USGS Site Area Geologic Map of Day, Potter,

Dickerson, Sweetland, and Sanderson. I believe the map data are very accurate, because they consistently make smooth surfaces and match boreholes closely.

A bad map would do neither.

SCHEDULE NOTES: In planning, we were to have had 16 weeks to perform this activity. Because of delays in the USGS borehole re-evaluation, we only have a total of 4 weeks. Both periods (16+4) are in addition to 4 weeks of review. This severely cramped schedule leaves us with little time for problem-solving and no margin for error. I believe, however, that the testing done and lessons learned in GFM2.1 will directly contribute to our ability to construct a valid and technically good model.

The late USGS data has another effect — the original plan called for direct USGS participation in model construction. But their own delays have cut them out of the picture and relegated them to — if anything — reviewers. I anticipate some harsh comments.

2/14/98 cont'd PLWEC

from them concerning our interpretations in this model. They will question the qualifications of myself, Elayer, and Hinds to make interpretations of Yucca Mountain volcanic units. They will cite obscure (sometimes undatable) documents that show contrary interpretations.

I counter that 1) the 3 modelers are capable geologists with more combined experience than the two in USGS, 2) any 5 geologists will, given the same data, make at least 6 different interpretations, each one valid, and 3) the USGS has a responsibility to provide beforehand any applicable DATA they are aware of.

This model is one of many possible interpretations. We strive to have all data and to make as robust a model as we can.

Any model that honors all known DATA (not other interpretations) must be considered valid.

GRIDDING NOTES

Earthvision software uses a "minimum tension" algorithm for gridding data (that is, for passing a surface through each datum). My tests show that this method produces a maximum misfit to Yucca Mtn borehole data of 0.2 feet. Typical fit is ± 0.02 feet. Volcanic deposition and erosion are "minimum tension" processes - that is, they follow paths of least resistance and tend to remove abrupt changes.

Constraining ^{the ~~use of~~ ~~the~~ ~~algorithm~~} to produce the desired results takes a) practice, and b) an understanding of how it works. In general \rightarrow

2/4/98 cont'd RUC

the algorithm works best when input data are evenly distributed across the entire map area. When the interpreter wants to constrain the location a slope of an abrupt change, she can make certain lines or data points that are close together. Providing too many constraining parameters often produces what we've called operators' when the algorithm struggles to match all inputs.

Minimum tautness, by nature, produces a statistically robust and generic interpretation. My approach to all cartography is, therefore, to use a gentle hand and "let the data speak" by not over-constraining the surface generating algorithm.

FAULTS: Adjusted the Paintbrush, Fox Ridge, and Midway faults according to comments from St. Dickerson (1885). These comments lead to minor adjustments in dip and changes in offset.

2/5/98 RUC

Fine-tuned the base TDR reference horizon. Adjusted the TDR data to fill in where no data are available. Did this by varying its thickness to 644 and adjusting to be consistent.

Encountered a question regarding some 1865 structural input. Offset of Sottawa fault is ~1500 feet at basehole WT-10, but is 520 feet or less at the SW corner of the map/panel area. The relation just WT-10 is a hole, which is an issue due the same offset + wiggle or before adjusting it in the model. Another possibility - low obliquity - is that the Sottawa fault had another, steeper, fault or crest →

2/5/98 cont'd RWC

under the alluvium. The existing scenario can be readily explained by ascribing the southward decrease in *pelitaria* aspect to the 3' NW-striking faults that intersect it right in that area — the 3' faults take up some of the aspect.

I reviewed the first few maps from Jennifer Hinds, and they look all right — no comments.

SQR for EARTHVISION v4.0 was approved today!

2/6/98 RWC FRIDAY

Reviewed Elayer's Topograph inches with him, and entered them into Earthvision by hand-digitizing.

COMBINING DATA: To use both borehole and measured section data in creating inchare grids, I use the graphic editor to copy meas. section data into my interpretive data file. Then

I use the formula processor to combine the interp file with the borehole file. Here's some sample names, using b4:

i3b4.dat Thickness (isobae) data from boreholes

x3b4.dat " " " from measured sections

i3b4RWC01.dat All data combined with my interp data

i3b4RWC01.dat My interp data only.

For final editing, I edit the i3<name>RWC01.dat file.

Started a horizon grid job to test/check all inchares down to base Calico.

} RWC

2/7/98 R/W/C SABBOTRY

Evaluated first-pass model.

302 Faces has everything to base Calico, just sand of reviewers' inches. PROBLEM AREAS: Geologic map mismatch at Busted Butte, The Prow, and NE of Yucca Wash.

Colored & studied the geologic map for clues why the mismatch. Concluded the following:

- 1) Need to end all lithophysical zones at Yucca Wash. North of YW, use only Tptm, Tptf, Tptpn, and pvl-3. These are defined in measured sections, and the ttpf break is on maps south of YW. Lithophysical zones can NOT be correlated to Φ boreholes.
- 2) Missed map contacts: a) bt4 on east side of Busted Butte; b) Tpcp west of The Prow; c) base Calico west of The Prow.
- 3) Dips under Alice Ridge are to the South.
- 4) East-dipping fault on E. side of Busted Butte (or equivalent) continues northward between Alice Ridge and WT #15, ~200 ft offset.
- 5) Need to better match dips at Berryman Point, The Prow, and NE corner.

Edited and fixed the data files involved in each of the above.

2/8/98 SUNDAY R/W/C Yes, I'm working through the weekend!

More map-matching.

Edited the bt4 structure surface to fit map data in the NE corner.

Implemented the Tpt zero-thickness line at furthest NE corner as indicated on the geologic map.

2/9/98 Monday RWC

Curious why so many measured section numbers seem far out of whack, I dug into the USGS publications and found some explanations. a) A couple of typis in my transcription; b) a couple of typis in their documents (trv2+3 are transposed in section Tpt-2); and 3) some numbers are minimums due to covered contacts; and 4) Tptf was misnamed Tptpm in section Tpt-1. Let USGS know of typis.

Remade the meas. section data and began re-mapping. Will pass on to Eloyer and Hinds.

bt3-Tpx-dc: I inquired over the phone to Jeb Dickerson, the USGS authority on the geologic map north of Yucca Wash, about these units. With his approval, I will make the chert of Delirium Canyon "look like" the extension of bt3 north of Yucca Wash. These units are rough lateral equivalents spatially, but are distinct eruptive units. This solution is a good one to allow the model to match the map north of Yucca Wash.

Incorporated Jennifer Hinds' interpretations, and gave the resulting data files the "02" designation.

Created the bt3/dc isochore map using the geologic map as a guide.

Structure of NE block: Try this: 1) Export top Calico; 2) Export ASCII data; 3) re-use as Ref Horizon; 4) edit only NE block by entering map contact data.

Started a horizon gridding job for evaluation.

2/10/98 92 WRC TUESDAY

Worked on btt reference horizon, tracing to get

units to match the geologic map.

Made some cumulative thickness maps for Job Elyria,

as he works on Topogob some thicknesses.

2/11/98 92 WRC Wednesday

Developed a method to keep five reference horizons separated by the desired amount.

1) Using the digital geologic map with elevations, d plotted the vertical separation of Top and Tpbtt.

2) Hunt-contoured these data to cover the entire area.

3) Made a 2D grid of the sp-bt thickness. 130p btt 2grd

4) Used this grid to take my interpreter btt contours

(S3BTRWMC03.dat) and produce new contours at sp

5) Deleted these interpreter contours near map along

data points where they may cause griding errors

6) Input to the sequence file (which contains the modeling

parameters) = sm3topp.dat (map data) and as "Helper"

data, S3TpepAIC.dat (the calculated new contours).

This method produced excellent results in a test model

using only three two units

Updated version 03 horizon grids to run overnight.

Yes, I left this blank on purpose!
92 WRC 02/11/98

02/12/98 Thursday TRLW=C

Evaluation of version 03:

- Bumps at tail of fault "imb"
- Need to somehow account for some short mapped faults that cause mismatch with geologic map:
 - ridge north of Alice Ridge;
 - ridge NE of WT#15;
 - between iron W2 and iron W3.
- bt units²⁺⁴ are all too thick at Busted Butte.
- a few bt⁴ wobbles near benches

Base TIVA Ref Horizon:

Removed some outcrop map contacts where minor faults cause misleading warps in this surface. Includes only spots at The Picou and the complexly faulted south-central part of the area.

Adjusted fault offsets for consistency - Windy Wash, Fatigue, "win-j-fat", and west Fran Ridge.

Can't match all map points because of faulting west of The Picou, hill NE of WT#15, hill N of Alice. These would require addition of ~4 fault blocks that don't affect any critical geometries involving benches, tunnels, flow barriers/pathways, or any issue I'm aware of. Each fault block added causes an increase in computation time and therefore decreases my ability to refine and edit the model.

VERSION 04: All units. May be able to export top of Calico for Ref Horizon.

2/17/98 RLW=C Tuesday after a 4-day weekend.

Horizon gridding version 4 did not run completely, so I fixed a file name problem and restarted it.

2/18/98 RLW=C Wed.

Version 304 matches the geologic map to a satisfactory degree. Contains a rogue low data point for lot 4 east of Jutul Jutte, but looks otherwise good. More analysis later.

2/19/98 Thu RLW=C

The PALEOZOIC SURFACE (Tertiary-Paleozoic unconformity) provided by LBNL geophysics group was constructed as a purely geophysical interpretation, and no attempt was made to make a geologic interpretation. This was discussed in a videoconference yesterday with the LBNL staff (Mark Feighner, Jan Daley, Lane Johnson, and others). I am helping them now attempt to make a geologic interpretation that can be used in the GFM. The geophysical interpretation is untenable in the model.

Version 305: • Fixed a fault offset polygon that was too small.

• Made Calico 1500' thick at NE corner on advice of Bob Dickerson (USGS mapper). • Smoothed "imb" fault to (hopefully) avoid lumpiness.

Started the horizon gridding job tonight. Objective is to export a usable Calico surface to make into a reference horizon.

} Blank RLW=C 2/19/98

2/20/98 RWSC Friday

Had to restart the version 05 horizon griding because I accidentally left some Bow horizon left as "the" instead of leaving them out, and the job failed.

Edited Rainbow Fault to represent the correct bend at Bow Ridge and back to p11 as an anomalously steep segment on an otherwise north-trending, moderately dip slightly listric fault. The fault to be used in version 06 is called "3300ft RWSC02.2.grd". A cross section through Bow Ridge has always bothered me as unrealistic because it had a steep bend in the Rainbow at p11. This edit makes the fault here more realistic; another change is to edit Edited Bow Ridge and Mistyox faults to remove some complexity that is not needed.

2/23/98 RWSC Monday

Version 305: Still needs edit to the reference horizon.

Adjusted east of Great Falls to match USGS cross section.

Adjusted above Somersung fault to correct a reversal of offset because of dip only there and dip still calling it 305.

Method: Created sequence files for each fault block making editing and horizon griding. The copied the revised files to the Vmaster horizon directory (called "horizon305").

Version 306: Used results of 305 as input to reference horizon for Calico. Griding only up to Toppen as a test.

RANK RWSC 2/23/98

Changes not requiring wholesale revision are given 1, -3, or a.b.c. numbering.

2/24/98 TUES

306 results: Unsatisfactory. The TptEn - the highest

surface built up from the Calico and bryozoa - impinges

on the north shore. Cause: Inadequate input control

Solution: Instead of inputting my own contours, I'll mix

the gull contours file output, with modifications where

needed. Call it version 306-2 (there is no 306-1, only 306 and 306-2

Main input: SC3TAC305EXRWC02.dat

Additional input: SA3TAC.dat, beholes and outcrops

306-2 results: Unsatisfactory. In several locations, the

Calico points cause bumps or connections across faults.

Solution: Create buffer zone polygons around the faults

and delete points inside the polygons. Polygons called

"S3TACBUREER.poly"

2/25/98 TUES Wed

306-3 results: Very good! So, results from surface to Calico

are good.

Spent the rest of the day conducting a Paleogeographic

Palaeozoic: More precisely, the Tertiary - Paleogeographic

The surface provided by LSL from gravity inversion in

unavailable. It matches no faults or thickness trends

Solution: Until a better surface is available, I have to

use one of my own interpretations.

Basis: The broad trends and depths from the gravity

inversion, matched with fault depths. Using only the

depth from geologic maps, I construct a Paleogeographic

surface that also satisfies the general gravity

Thank GWFC 2/25/98

2/26/98 RLW=C Thursday

Began incorporating the final lithostat borehole contacts from the USGS borehole re-evaluation activity. Evaluation: With the exception of one type, the new corrections seem to reduce the number of anomalously thick or thin intervals. USGS corrected the type.

2/27/98 RLW=C Friday

Requidled horizons down to Calico. Exported and edited Calico. Began new horizon gridding job for all horizons.

3/2/98 RLW=C Monday

Gridded horizons down to Trambt, but results were bad because I specified the older inchores files instead of the newer. This happened because I copied an older .seq file and failed to edit it. From now on, I'll use only the most current .seq file and will edit before each run. This is version 307. RLW=C

Requidled Calico to Trambt to export as new Reference Horizon @ Trambt. Need this horizon to constrain fault effects, especially Paintbrush.

3/3/98 RLW=C Tues

Re-edited Crater Flat Gray units (inchores) to produce more consistent interpretations. Based on examining the results of version 308.

BLANK RLW=C

versions
308a-c
2/12/98
3/14/98

3/14/98 RWL

Wednesday

Continued editing + reworking Cret. Plat (P) in several sections, as Jim double-checking the data and the washer grids to make sure they're defensible. By consolidating the washers to produce consistent intervals. Dan also summarizing the "bumpiness" produced by abrupt change upon abrupt change. Version: 308d

3/15/98 RWL Thursday

308d evaluation: Very good, with the exception of the following trouble spots.

- 1) fault block "below A1" - there's a mismatch between horizons built down from b14 and those built up from Calico. Solution: Build a partial model in only that fault block and copy the results to the model.
- 2) Persistent bumps of unknown origin beyond SE termination of "sub" fault. Solution: Try bending fault to more E-W orientation. Could try doubling grid size for de grids, but this would double computation time without increasing accuracy.

3) Steeping in fault block "above Drilling" caused by irregularities in b14 contour data, caused by minor faulting. Solution: Smooth in b14.

4) Presence of horizons below Toplin - ^{308c} ~~308b~~ "above Spohn" - Solution: Plot contour points to Calico and "above Spohn" - Solution: Plot contour points to Calico

Work on these will be done over the next several days during + after our company's annual training offsite.

3/5/98 cont'd RW=C

Source of error at breches: Some breches contain

no geological log about 300 feet or above the Topog Spring Tuff. These include the "c" holes and b#1, H-1, H-6, G-2, and possibly another 1 or 2. Without the density log, we can not confidently calculate the rock units in these holes' tops to the other breches; therefore, we decided not to use the non-Q, other

information in these intervals (lithologic logs). We have found that the old lith logs introduce error and variability. In a couple of these cases, there is also no lithologic log data because the holes are cored.

The result is: these holes do not tie to the primary reference horizon at BT4, and all thicknesses above the available density logs are interpolated (imposed) using the other breches. The net result is a possible mismatch between model elevations and breche elevations

there should be a bulk drift and relatively constant thickness of the logged intervals were used. Each hole is tied to the Colico reference horizon, and the error is taken up in the Topog unit.

Geologic Source of Error: Some breches contain minor faults that cause apparent thickness anomalies, or even cut units out entirely. Examples are RW#1 and WT#1. These faulted units are extremely difficult to model precisely.

The solution to these errors would be to build the model tentatively to make each horizon a reference horizon. This would require approximately 16-20 additional wells, which is prohibitive in the current project schedule. Impact: Minimal; nearly within

Case 2: Original geologic interpretation; that #1 penetrates the Paintbrush fault into the Paleozoic carbonates. - Robert 2/10/98

3/6 - 3/8/98 No activity TRLWC

3/9/98 TRLWC A side study: VSP interpretation by LBL. To test + evaluate the seismic studies of VSP and reflection at borehole #1, I'm creating submodels around that borehole.

Case 1: #1 is on the down side of Paintbrush fault. This is the interpretation favored by the LBL geophysicists.

Problems: Requires 80°-85° dip of Paintbrush fault, which map data indicates dips 50°-70°. Brings Paleozoic to elevation of ⁴⁶⁰ ~~460~~ ft beneath Fran Ridge, which is near the base of the Tram Tuff - unprecedentedly high in the stratigraphy.

Conclusions: The LBL interpretation is permissible if the interpretation of a fault at Pz in #1 is interpreted another way. I prefer the original way (Case 2) based on the thinning of lower Tertiary rocks and evidence of faulting in borehole #1. I'll provide the alternate model as a possibility. ^{RLWC 2/1}

3/10/98 TRLWC Tuesday Back to GF13.0

Examined the base Tiva reference horizon in anticipation of reviewer comments, and adjusted some fault offsets to make them more laterally constant (as appropriate).

These places include upper Drillhole Wash and the "top" fault. Re-routed the buried Drillhole Wash fault at the far NW end to separate offset outcrops.

3/11/98 - 3/19/98 No activity: Technical Review in progress. TRLWC

Review by OAR-5TH procedure, "Review of Technical Documents and Tests".

Review package will be submitted to records center; search for "GF13.0" ^{RLWC 4/198}

3/20/98 Friday ZLVC

Incorporated USGS aerials comments in isohone grids and updated isohone griding. Changes are mostly

interpretive regional trends, but the USGS also used

the opportunity to edit their borehole data.

And as the ^{borehole} changes are substantial (many open boreholes

only). These changes will be submitted as part of their deliverable

of re-evaluated borehole that contacts (a Q process) ZLVC also

3/23/98 Monday ZLVC

Debugging: Requested two fault blocks to correct reference

borehole apertures along fault lines and identify

3/24/98 Tues ZLVC

Continued debugging (fixing problems). Version 3094

media b44 and Colico adjusted in fault blocks "behind"

"below Splay N, and below DILLINE" where boreholes p#1,

G-1, and UZ-1 collar at a below b44. To find the

projected elevations of b44 at these holes, I projected the

thickness from Colico to b44 (for p#1), and estimated b44

elevation from the geologic map & borehole logs (G-1, UZ-1).

Requested these fault blocks.

3/25/98 Wed. ZLVC

Version 3098 in the first to include pre-Colico zones

once the version. Need to adjust deep apertures of b44,

imb, northern Bouthwick, northern Fajeno faults, apertures

one much better than anticipated. Also, p#101 & 1

Yasca and Feb top one much better than anticipated.

Version 309C: includes typed fault blocks from yesterday.

quite good, lacks correct fault apertures at deep boreholes.

3/26/98 Thurs. RWC

Job running all day: Horizon gridding from the Calico reference horizon. 2⁺ horizons per block, 12-13 hours total run time.

NOTE: Fault block "above DrillNE" extends down only to lower Topopah, so the lower Topopah units in this block can NOT be built upward from Calico.

Bought a laminator today just so I could write something extraneous here.

309 D.F.E. DIVE 06/98

3/27/98 FRI RWC

Fixed the horizons in "below Bow". Source of problem: Tacbt was given same thickness as Tac by my own typographic error. Just need to double check everything and use proven sequence (parameter) files.

"309F" Evaluation: Just a few spots left to fix: rollovers of "Turd" in hanging wall of Bow, Midway, and Paintbrush faults; a few lumpy spots in Tac and Turd.

Version 310 is intended to be the final model, with the corrections of 309F. Everything will be regrided so that ties across dying faults can be sewn up by the software.

3/30/98 Mon RWC

310: Need to fix: Geometry + offsets at "Forty" and "East" faults — "Forty" must be historic to have "East" as a conjugate.

Could not completely fix horizons in Bullseye + lower in fault block "above East" between 759,000 - 774,000 ft. Nothing. The fault block's narrow bottom wedge does not allow proper calculation of horizon grids.

3/31/98 Tues. RLV-C

Filled fault block "above Drilline" from the top -
ref horizons at Tac and Tund are below the blocks.

Fine-tuned the Paleozoic surface for accurate
fault effects as per USGS review comments (QAP-STEP2 review).

Constructed the surfaces for alluvium, post-Tina North,
and Tina-Rainier at grid size 371x491 for better
accuracy and detail.

The final faces file (gfm3.faces) looks good.
I'm satisfied that this model is as good as I can
get it at this time.

Known Problems: A couple of fault blocks became
so narrow at their wedge-shaped bottoms that I can
not control the horizons' grids there. Unfortunately this
includes the block between the Drillhole Wash faults,
which figures prominently in many maps + cross sections.

Data + Model submitted to Numerical Model Warehouse
on 3/31/98

End of Activity for Geologic Framework Model

Blank RLV-C

I initially reviewed this notebook on 6/3/98 and discussed the review with Robb Clayton on 6/8/98. As a result of this discussion, Robb added several explanatory notes to the notebook. I reviewed these notes on 6/12/98 with Robb and now find the notebook for 15M3.0 to be acceptable.

Jeff M. S. Cleary
6/12/98

PART II:

Integrated Site Model ISM3.0,
Integration of Rock Property and Mineralogy Models

25 August 1998 RJC

Received the output from Chris Reardon's (Sandia Lab)

rock property models a few weeks ago, on CD as well as the technical data base. The output consists of

property values at grid nodes only - no x, y, z coordinates. Each model is accompanied by a file of grid specifications -

actually, one file for all - specifying grid coordinates, size, and spacing.

Using this file I updated the spot models into the GFM3.0 in Cartesian format. Ran into problems

when I specified the very grid size - the input only works when the spot are correct. This process is

surprisingly simple and fast - I completed all 15 model inputs in a few hours.

The input functions like this: Property grid node values are assigned x, y coordinates and modeled in Cartesian

to get inside the specified rock layers. The resulting files are Cartesian binary 3D grids, one in each fault block.

To summarize, I then create a "layer" file for the model

very. The Cartesian-format model is an exact reproduction of the SWL geostatistical model except it

is now precisely fitted into the geologic model. I sent several graphics to Reardon to check,

and he replied that the process appears to have worked correctly.

RJC

8/25/1998 cont'd TRW=C

I am attempting to quantify uncertainty in the geologic model to determine the impacts of SD-6 and WT-24 strat contacts on GEM3.0. I've developed an empirical approach based on a) field and bench observations, and b) contouring variability. In the field we can observe lateral thickness and/or elevation changes of 10 feet over 200 feet (e holes) or 30 feet abruptly (Miller Ridge). In creating maps for GEM, contouring uncertainty is approximately ± 50 feet at 2000'-3000 ft from data. In other words, contours can typically be drawn $\pm 50'$ in areas more than ≈ 2000 feet away from benches, without any real constraint to determine exactly where that contour needs to be.

Using this empirical relation, I calculated a minimum distance grid in which each grid node value was equal to its distance from the nearest data point. I then divided that grid by a factor to obtain values of approximately 50 feet at 3000' from nearest data.

Results: So far the resulting map appears to reflect what I would have expected from experience ^{with} with the model and data. I cut off values to be no more than 50 feet, at least for this first pass, to avoid values going extremely high. This map probably only applies to areas of interpolation - areas of extrapolation are difficult to quantify. The map will be in the ISM3.0 report.

I spent much of the previous weeks writing the GEM portion of the ISM3.0 report.

} TRW=C

8/26/98 RWFS

I received the mineralogic model output from Bill Carey at LAMM by electronic transfer. The file appears to be complete and correct as described.

8/27/98 - 9/7/98 No activity RWFS

8 Sept 1998 RWFS

Began a "jack knife" uncertainty analysis. The idea is to begin with one set of brechels to predict the next, add in the second set to predict the third, and so forth. By plotting the brechels misfits (predicted versus actual) we get a measure of predictability, a uncertainty. I chose to do the jack-knife on the Toppek leaves vitrophyre (Tppv3) because it is a critical boundary for repository design, and ~~is~~ assessing its predictability is important.

First Jack-Knife: "Black box" approach, letting the minimum tension algorithm make predictions. I included outcrop data, since the quantum of interest is subsurface uncertainty.

Results: The average absolute value of predicted minus actual asymptotically approaches 30-40 feet, and the median approaches 30 feet.

Analysis: These values agree exactly with my "bone game" estimate of 50 feet using bond-centering to see how much "play" there is between epithermal brechels. I had estimated that we can't predict closer than 50 feet where brechels are 300 feet away from the spot we're predicting. WT24 and 5D-6 support this range.

9 Sept 1998 RWFEC

Second Check-Kaife: Proholes plus interparticle contact. This is a closer approximation of how GMS was built.

Results: The average prediction error levelled off at about 39 feet for the TPTPS vitrophyre. This is consistent with my estimates from manual contouring, and so I have confidence that it's about right. Using interpretation (geologic reasoning) cut the average prediction error from 79 feet down to 39 feet. My GMS3.0 progresses for SD-6, WT-24, and the cross-block drift have been within this window.

10 Sept 1998 RWFEC

Mineralogy model via 3D grid has been calculating for ~60 hours now. I contacted Jill Casey today to get their mineralogy model divided up by strata so this process will hopefully work better.

15 Sept 1998 RWFEC

Further testing to see how I can most efficiently build the mineralogic model.

I split the LAM data by horizon and grouped by the same "rock property" unit groupings used for the rock property models. Then used this as input to a model. Still takes >24 hours to make a model.

So I've asked Derek Taylor at Dynamic Graphics for ideas.

Working on the ISM3.0 report and other projects, not full-time on these models, so may not have entries every day.

18 Sept 1998 TPLWSC

Each numerologic panel file takes about 3 days to run, so Dave prioritized them to run before I get a better reaction from DGL. I'll make Calvo-Bowl queries, DSW capabilities, and AT results. These are investigations only; the models (mostly one what was completed at LML). I do not want to calculate them, only draw contours through them.

24 Sept 1998 TPLWSC

Finally completed the 3 minimal form
Thought: GEM30 uses same data which are not "directly" related on to address safety and waste violation issues, but which are needed to flesh out the model and fill out the boundaries. The intent of the form at present is to qualify all data which are "directly" related upon... I use the other data as well for reasons not important to safety & waste violation. I suggest grading these data at a level below the "directly" related upon case.
Work on the ISM30 report and figures continues after this date.

— End of ISM30 Scientific Notebook —

— TPLWSC — BT

As doc is read on the affords
Series of e-mail correspondence, I
(JES M: Cleary) completed a review of
part II of this notebook (starting on page
24) on 11/20/98. This review was
accomplished with OAP-5111-3 in order to
re-review of the first part of the

 Norma Biggar
01/28/99 01:13 PM



To: Robert Clayton/YM/RWDOE@CRWMS, Andrew Burningham/YM/RWDOE@CRWMS
cc:
Subject: Re: Scientific Notebook Review - ISM3.0

This string of memos covers all comments that robb was referring to. I'll give Robb a copy of the Scientific Notebook compliance checklist.

Forwarded by Norma Biggar/YM/RWDOE on 01/28/99 01:07 PM

 Jeff McCleary
01/19/99 01:58 PM

To: Norma Biggar/YM/RWDOE@CRWMS, Robert Clayton/YM/RWDOE@CRWMS, Darrell Porter/YM/RWDOE@CRWMS
cc:
Subject: Re: Scientific Notebook Review

Norma, Robb, Darrell,
The attached correspondence gives the status back in November, and I guess that is still the status. I am sympathetic to Robb's rationale for not including the "Q" status in the notebook, and I would certainly accept a short discussion in the notebook that explained the situation and referenced the pages/tables/figures in the report where the "Q" status is indicated, but I still feel that the requirement can't be ignored. The notebook has to at least indicate where the information exists and why it is not in the notebook directly.
Jeff

 Jeff McCleary
11/23/98 08:39 AM

To: Robert Clayton/YM/RWDOE@CRWMS
cc: Norma Biggar/YM/RWDOE@CRWMS
Subject: Re: Scientific Notebook Review 

Robb,
You raise some valid points, and I agree that given the situation there is no point in going into much detail in the notebook. On the other hand, given my recent audit experiences, I am becoming an ever bigger fan of explicit statements in notebooks and reports relative to any procedural compliance issues. What do you think of this idea -- include a statement in the notebook fairly similar to what you have written here. State that the "Q" status of data is listed in table _____ of the report, and that is current as of some date. The mineralogic part of the ISM is non-Q and the rock properties Q status is indeterminate as of some date, but these are subject to changes beyond your control. That type of short discussion would be consistent with the sort of comment on "directly relied on" that you have on page 28. I guess the mechanics would be that I would write a review comment that there should be a more explicit statement on the Q status of the various model components -- you would respond with the short discussion that I'm proposing -- then I would sign off on the review. That should leave a clear trail for any later audit. See what Norma thinks and get back to me.
Thanks,
Jeff

To: Jeff McCleary/YM/RWDOE@CRWMS
cc: Norma Biggar/YM/RWDOE@CRWMS
From: Robert Clayton/YM/RWDOE
Date: 11/23/98 07:58:05 AM PST
Subject:  Re: Scientific Notebook Review

Jeff,

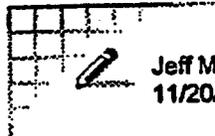
For the identification of QA status of data, I've always been relying on the report, not the notebook. I never thought of that as a significant part of the notebook. For the ISM3.0, that list is 3-4 pages long. The QA status of those data is in flux, and has been all year as geophysical logs are [still being] reviewed. So any information I'd put in the notebook would be subject to change.

While I was completing the notebook, there was still some question as to the QA status of the mineralog and rock properties models. It turns out the Mineralogic models are non-Q (software and data) and we're not quite sure yet about the rock properties models. Since those issues are really out of my hands and are subject to the findings of audits and other scrutiny, I'm not sure it's such a good idea for me to say in my notebook what the QA status of someone else's model is. I could say what I know about it, but what would happen if I say it's Q and it turns out not to be? Would my notebook then be used to discredit the ISM process?

I'll be happy to take care of your comments in the notebook.

— Robb —

Jeff McCleary



Jeff McCleary
 11/20/98 02:50 PM

To: Norma Biggar/YM/RWDOE@CRWMS, Robert Clayton/YM/RWDOE@CRWMS
cc:
Subject: Scientific Notebook Review

Norma and Robb,

I completed my review today. I decided to re-read the whole thing to refresh my memory and also to look at things in light of the recent audit and data traceability issues. I think we are weak in the area of identifying "Q" and "non-Q" data sources. There is no mention at all as to whether the rock properties and mineralogic models are "Q" or "non-Q", and the distinction is there but somewhat buried in the rest of the notebook. The procedure only requires that "non-Q" data be identified, but I would recommend, for the sake of clarity, that you provide a list of data inputs and their "Q" status. If that is too cumbersome, just simply list the "non-Q" data and state that all the rest are "Q".

Robb — take a look at page 17, should the "Version 08d" at the bottom of the first paragraph be 308d? On page 19, should the "(case 1)" in the middle of the page on the right side be (case 2) [the original interpretation as written sideways near the top]?

I also re-read the procedure just before I did the review and other than a more explicit identification of Q and non-Q data I think it is in good shape. Let me know if you have any questions.

Jeff

note back and resulted in identifying that
 the 2 sites of model component was not
 adequately addressed. Their errors were
 also noted on pages 17 and 19. Following
 some correspondence (see e-mails) the PI
 added explanatory material on page IV and
 corrected the errors on pages 17 and 19.
 I reviewed these addresses/corrections
 on 3/17/99 and now find the
 notebook acceptable.

M. J. Day
 3/17/99

With the publishing completion of the present network model
 engineering approaches, rigorous, formal, model compliance
 and technical content, the present network is approved for
 submission to the Reader Learning Center

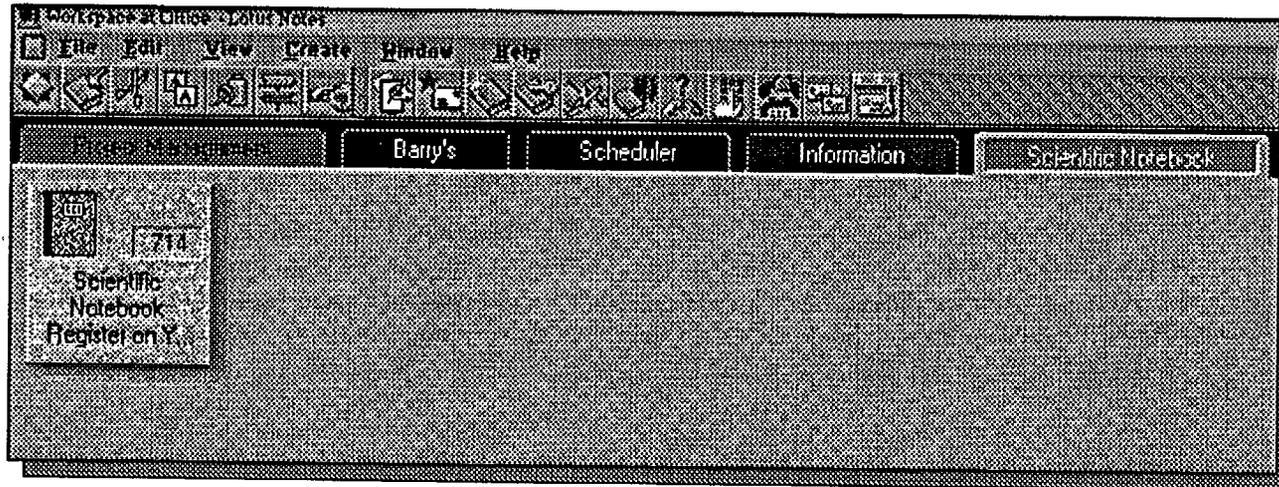
Thomas P. Papp 3/31/98

***The Control and Use of
Scientific Notebooks for
OCRWM Activities***



Scientific Notebook Register

Scientific Notebook Register



Instructions for Scientific Notebook Register

For any corrections or questions concerning this database Contact Darrell Porter.

Getting Started

The first screen allows the user to read the file with sorting options. The "**CREATE NOTEBOOK**" button also allows the creation of a notebook identifier. For other tasks of extending a notebook into a new volume or closing a notebook follow the instructions below.

Important Note: It is not possible to create a number of choice. Upon creating a notebook identifier, the computer always gives the next higher number under the given ALPHA code.

Hints

You may press the ESC key at any time within a Document to leave without saving. If the Save Dialog appears just click on the button labeled "No". You can press the Tab button to traverse down the fields, and the Shift and Tab buttons simultaneously to traverse up the fields. When choosing a record from a view, double click on the record with an arrow pointing to it, everything else is just a category header. These categories can be collapsed or extended by using the buttons in the action bar, which is located just above the viewing area.

Creating a New Scientific Notebook

From the Main Menu click on the button label "Create Notebook".

Completing the New Scientific Notebook

You must choose an organization and subdivision before continuing.

After both organization and subdivision have been chosen a button labeled "Create a New Scientific Notebook will appear on the bottom of the form.

After clicking on this button six new fields will appear.

You must complete everything on the form except the WBS Number before you can save the form.

Saving the New Scientific Notebook

After the completion of the form you may click on the button labeled "Save Notebook" which is located above all of the fields.

Extending a Scientific Notebook

Choose one of the listing (e.g. List By XXXXX).

Select a notebook to be extended and double clicking on it to launch it.

(NOTE: The record to double click on will have an arrow pointing to it, everything else is a category)

You should now see a completed form with two buttons above the fields labeled "Create New Volume" and "Close Notebook". Click on the "Create New Volume" button and the form will go into an edit mode.

(NOTE: You must be the original author of the document to extend it, unless you are an editor or above)

Notice all of the fields except the date the notebook was opened and the notebook title are now blank. You will be required to complete the entire form with the exception of the WBS number field.

Saving a New Volume

After completing the form, you need to click on the button labeled "Save As New Volume" which is located where the "Create New Volume" button was prior to pressing it.

Closing a Volume of A Scientific Notebook

From the Main Menu Button labeled "Opened Notebooks" double click on the Notebook you want to close. You should now see a completed form with two buttons above the fields labeled "Close Notebook" and "Create New Volume". Click on the button labeled "Close Notebook".

Completing a closed notebook

All fields must be completed, except for the description, which is located at the bottom of the form.

Saving a Closed Scientific Notebook

Click on the button labeled "Save Closed Notebook."

Help

Logout

CREATE NOTEBOOK

LIST BY TITLE

LIST BY NOTEBOOK ID

LIST BY AUTHOR

LIST BY STATUS

LIST BY PARAGRAPH

DESIGNERS VIEW

REVIEWS

FULL LISTING

NO COMPLIANCE

COMPLIANCE ONLY

FULL COMPLIANCE

▲ 00376:E-20-43/44
 ▲ AUTHOR: ROY, AJIT

▲ LA-EES-1-03-94-006: HIGAKU XRD ACTIVITIES
 ▲ AUTHOR: KUK, E.
 + Volume 1 SN:LANL-SC-098-V1 Closed: 11/11/99

▲ LA-EES-5-NBK-90-020: BUSTED BUTTE ON-SITE LOGBOOK #2
 ▲ AUTHOR: BUSSOD, GILLES
 + Volume 1 SN:LANL-SC-039-V1 Opened: 10/06/98

▲ TWS-EES-1-5/06-18: NNWS 1 LOGBOOK
 ▲ AUTHOR: VANIKAN, DAVE
 + Volume 1 SN:LANL-SC-114-V1 Closed: 10/21/91

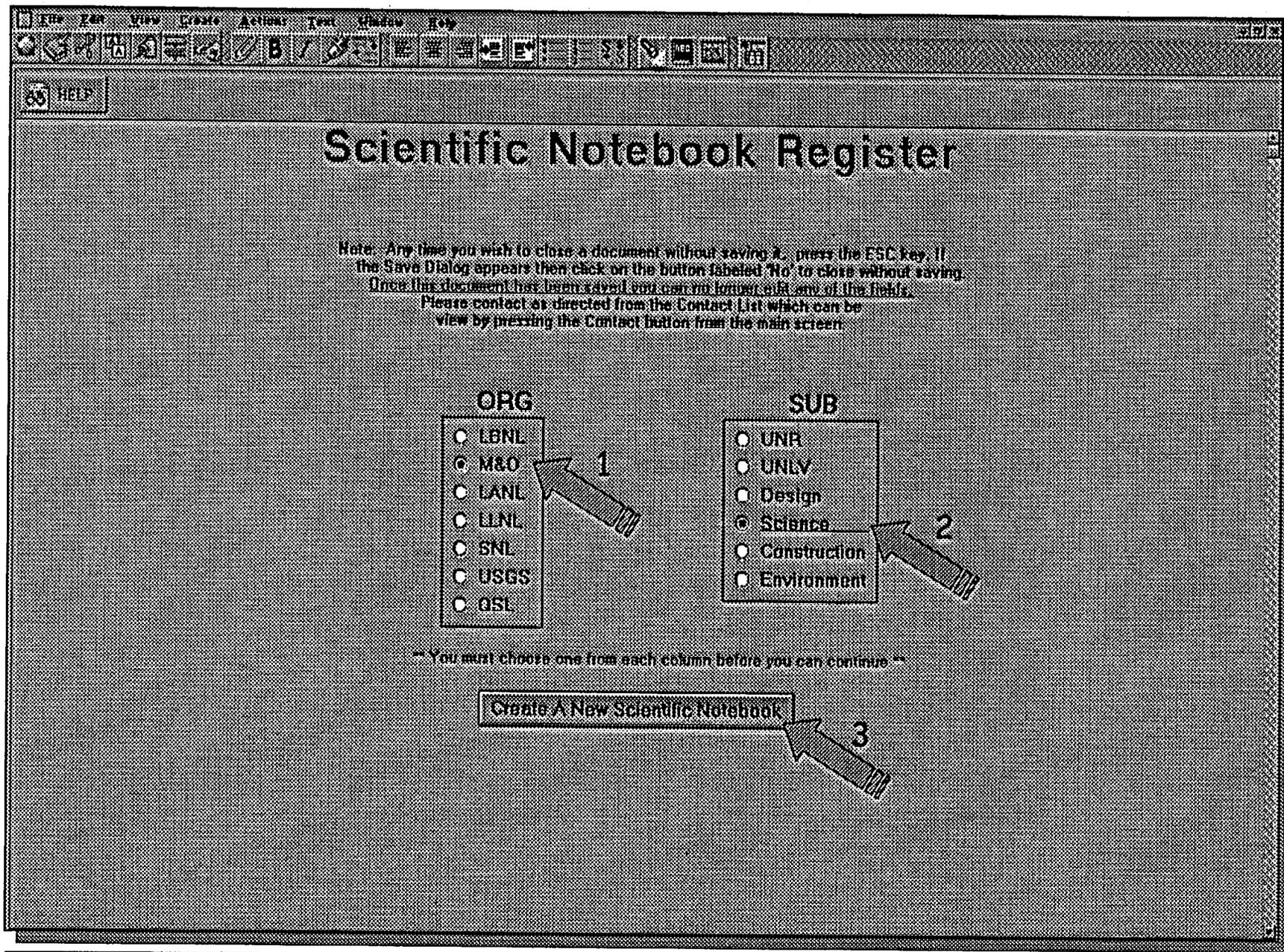
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