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**OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
ANALYSIS/MODEL COVER SHEET**

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Page: 1 of: 30

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OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
ANALYSIS/MODEL REVISION RECORD

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Complete Only Applicable Items

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1. PURPOSE

The purpose of this document is described in CRWMS M&O 1999b, and is to develop a predictive model for the diffusivity of ions in unsaturated media. The scope of this document is limited to developing a model showing how resistivity and diffusivity can be estimated as a function of water content.

2. QUALITY ASSURANCE

This document was prepared in accordance with AP-3.10Q, *Analyses and Models*, and the Development Plan (CRWMS M&O 1999b), which was prepared in accordance with AP-2.13Q, *Technical Product Development Planning*, and is subject to quality assurance controls. A Technical Change Request (T1999-0131) was approved in accordance with AP-3.4Q, *Level 3 Change Control*.

This technical document has been evaluated (CRWMS M&O 1999c) in accordance with QAP-2-0, *Conduct of Activities*, and has been determined to be subject to the requirements of the *Quality Assurance Requirements and Description* (DOE 1998a). The QAP-2-3, *Classification of Permanent Items*, evaluation entitled *Classification of the Preliminary MGDS Repository Design* (CRWMS M&O 1999a, p. IV-1) has identified the ex-container system as QA-2, important to waste isolation. Diffusive inverts are not specifically classified, but the invert is a component of the ex-container system. For this document, it is assumed that the classification of a diffusive barrier is QA-2, important to waste isolation. Also, the invert is part of the engineered barrier system, which the *Q-List* has identified as QA-1, important to radiological safety; and QA-2, important to waste isolation (DOE 1998b, p. II-9). The invert is not specifically on the *Q-List*.

This model is validated in accordance with Section 5.3 of AP-3.10Q, *Analyses and Models*. Model validation is discussed in Section 6.5. Qualified and accepted input data and references have been identified. No unqualified data were used in this report. All inputs are documented in Attachment I of this report in accordance with AP-3.15, *Managing Technical Product Inputs*. Results of this model have been submitted to TDMS in accordance with AP-SIII.3Q, *Submittal and Incorporation of Data to the Technical Data Management System*. Computer software and model usage are discussed in Section 3 of this report.

3. COMPUTER SOFTWARE AND MODEL USAGE

No software subject to the requirements of the *Quality Assurance Requirements and Description* (DOE 1998a) was used in the preparation of this document. The model developed herein is validated in Section 6.5. The developed model is appropriate for the estimation of conductivity and diffusivity. The results of this report are within the range of validation, as discussed in Section 6.5.2.

4. INPUTS

4.1 DATA AND PARAMETERS

4.1.1 Archie's Formula for Saturated Conditions

$$R_{sat} = A * R_{water} * \Phi^{-m}$$

$$R_{sat} = R_{water} * \Phi^{-m} \quad (\text{Eq. 1})$$

where:

- R_{sat} -Resistivity of saturated material
- R_{water} -Resistivity of water in the pore space
- Φ -Porosity
- m -Cementation factor
- A -Empirical factor, $A=1$

Source: (Keller and Frischknecht 1966, p. 21).

This equation can also be arrived at by combining the following two equations:

$$R_{sat} = R_{water} * f \quad (\text{Eq. 2})$$

where:

- R_{sat} -Resistivity of saturated material
- R_{water} -Resistivity of water in the pore space
- f -Formation factor

Sources: (Pirson 1963, p. 22; Bear 1972, p. 113).

and

$$f = \Phi^{-m} \quad (\text{Eq. 3})$$

where:

- Φ -Porosity
- m -Cementation factor

Sources: (Pirson 1963, p. 23; Bear 1972, p. 116).

Combining Equation 2 and Equation 3 yields Equation 1.

4.1.2 Cementation Factor for Unconsolidated Sand

The cementation factor for unconsolidated sand has been widely reported as 1.3.

Sources: (Bear 1972, p. 116; Pirson 1963, p. 24).

4.1.3 Archie's Formula for Unsaturated Conditions

$$R = R_{\text{sat}} * S_w^{-n} \quad (\text{Eq. 4})$$

where:

- R - Resistivity of unsaturated material
- R_{sat} - Resistivity of saturated material
- S_w - Fractional saturation, volume of water divided by volume of pores
- n - Saturation exponent

Sources: (Bear 1971, p. 116; Keller and Frischknecht 1966, p. 28; Pirson 1963, p. 24).

4.1.4 Saturation Exponent for Unconsolidated Sand

The saturation exponent for unconsolidated sand has been accepted by the scientific community as 2.

Sources: (Bear 1972, p. 116; Keller and Frischknecht 1966, p. 28; Pirson 1963, p. 24).

4.1.5 Nernst-Einstein Equation for Diffusivity

The Nernst-Einstein Equation is as follows:

$$D_0 = 8.931 \times 10^{-10} T \left(\frac{l_+^0 \cdot l_-^0}{\Lambda_0} \right) \left(\frac{z_+ + z_-}{z_+ \cdot z_-} \right) \quad (\text{Eq. 5})$$

where:

- D_0 - Diffusivity of molecule at infinite dilution (ionic pair), in $\text{cm}^2 \text{sec}^{-1}$
- T - Temperature, in K
- l_+^0 - Cationic conductance at infinite dilution, in S/equivalent
- l_-^0 - Anionic conductance at infinite dilution, in S/equivalent
- Λ_0 - Electrolyte conductance at infinite dilution, in S/equivalent
- z_+ - Valence of cation (absolute, i.e., no sign)
- z_- - Valence of anion (absolute, i.e., no sign)

Source: (Perry and Chilton 1973, p. 3-235).

$$\Lambda_0 = l_+^0 + l_-^0 \quad (\text{Eq. 6})$$

where:

- l_+^0 - Cationic conductance at infinite dilution, in S/equivalent
- l_-^0 - Anionic conductance at infinite dilution, in S/equivalent
- Λ_0 - Electrolyte conductance at infinite dilution, in S/equivalent

Source: (Perry and Chilton 1973, p. 3-235).

It can be shown that the square of the average of two (unique) numbers is always greater than their product (Attachment II).

The following statement will allow a simplification of Equation 5:

$$\bar{l}^2 \geq l_+^0 \cdot l_-^0$$

where:

l_+^0 -Cationic conductance at infinite dilution, in S/equivalent

l_-^0 -Anionic conductance at infinite dilution, in S/equivalent

\bar{l} -Average ionic conductance at infinite dilution, in S/equivalent

Source: Equation II-2.

It is conservative to substitute the average ionic conductance for the product of the cationic and anionic conductance because the resulting diffusion coefficient, if altered, will be made larger (i.e., a faster rate of diffusion). Incorporating this substitution and Equation 6 into Equation 5 yields:

Equation 5:

$$D_* = 8.931 \times 10^{-10} T \left(\frac{l_+^0 \cdot l_-^0}{\Lambda_0} \right) \left(\frac{z_+ + z_-}{z_+ \cdot z_-} \right)$$

$$\Lambda_0 = l_+^0 + l_-^0$$

Equation 6:

using conclusion from Equation II-2:

$$\Lambda_0 = 2\bar{l}$$

substituting:

$$D_* = 8.931 \times 10^{-10} T \left(\frac{\bar{l}^2}{2\bar{l}} \right) \left(\frac{2}{1} \right)$$

simplifying:

$$D_* = 8.931 \times 10^{-10} T (\bar{l})$$

$$D_* = 8.931 \times 10^{-10} T \left(\frac{\Lambda_0}{2} \right) \quad (\text{Eq. 7})$$

where:

D_* -Diffusivity of molecule at infinite dilution (ionic pair), in $\text{cm}^2 \text{sec}^{-1}$

T -Temperature, in K

l_+^0 -Cationic conductance at infinite dilution, in S/equivalent

l_-^0 -Anionic conductance at infinite dilution, in S/equivalent

\bar{l} -Average ionic conductance at infinite dilution, in S/equivalent

Λ_0 -Electrolyte conductance at infinite dilution, in S/equivalent

z_+ -Valence of cation *(absolute, i.e., no sign)

z_- -Valence of anion *(absolute, i.e., no sign)

*Note: This equation results in the highest diffusivity for ions with a valence of one, such as potassium chloride. In this equation cation and anion valences are taken as a value of one.

Note: The constant in Equation 5 is derived from the universal gas constant and the Faraday constant (Atkins 1990, p. 764) in the following manner:

$$R / F^2 = 8.931 \times 10^{-10} \quad (\text{Eq. 8})$$

where:

R -Gas constant, $R=8.31451 \text{ J K}^{-1} \text{ mol}^{-1}$ (Atkins 1990, front cover)

F -Faraday constant, $F=96485 \text{ C mol}^{-1}$ (Atkins 1990, front cover)

The Nernst-Einstein Equation defines a direct proportionality between equivalent conductance and the diffusion coefficient of an ion. Given the equivalent conductance of a solution of ions, the rate of diffusion can be found through the Nernst-Einstein Equation.

4.1.6 Equation Relating Equivalent Conductance and Conductivity

$$\lambda = \kappa / c \quad (\text{Eq. 9})$$

where:

λ - Equivalent conductivity (or molar conductivity), in $\text{S cm}^2 \text{ mol}^{-1}$

κ - Conductivity, in S cm^{-1}

c - Corrected concentration, in mol/L

Source: (Atkins 1990, p. 750).

4.1.7 Conductance as a Function of Conductivity

$$\kappa = G * \Theta \quad (\text{Eq. 10})$$

where:

κ - Conductivity, in S cm^{-1}

G - Measured conductance, in S

Θ - Cell constant, in cm^{-1}

Source: (Atkins 1990, p. 751).

Note: $G=R^{-1}$ (where R is resistance) and $S = \Omega^{-1}$ (Atkins 1990, p. 750).

4.1.8 Concentration Corrected for Activity

$$c = a * M \quad (\text{Eq. 11})$$

where:

c - Corrected concentration, in mol/L

a – Activity coefficient, dimensionless.

M – Concentration, in mol/L

Source: (Weast 1981, p. F-79).

4.1.9 Viscosity of Water at 20 Degrees Celsius

The viscosity of water at 20 °C is 1.002 Centipoise (Weast 1981, p. F-42).

4.1.10 Viscosity of Water as a Function of Temperature

$$\log_{10} \left(\frac{\eta_T}{\eta_{20}} \right) = \frac{1.3272 \cdot (20 - T) - 0.001053 \cdot (T - 20)^2}{T + 105}$$

Rearranging:

$$\eta_T = 1.002 \cdot 10^{\left[\frac{1.3272 \cdot (20 - T) - 0.001053 \cdot (T - 20)^2}{T + 105} \right]} \quad \text{Eq. (12)}$$

where:

η_T – Viscosity of water at temperature T, in Centipoise [gm/cm sec 10²]

η_{20} – Viscosity of water at 20 °C, in Centipoise [gm/cm sec 10²]

η_{20} = 1.002 Centipoise (4.1.9)

T – Temperature, in Celsius

Source: (Weast 1981, p. F-42).

4.1.11 Resistivity and Conductivity of 0.1 Molar Potassium Chloride

The conductivity of 0.1 molar potassium chloride is 0.012856 S/cm.

Source: (Robinson and Stokes 1965, p. 462).

The resistivity of 0.1 molar potassium chloride is (0.012856 S/cm)⁻¹ = 77.7 ohm-cm.

Source: The relationship between resistivity (R) and conductivity (κ) is: κ=R⁻¹.

Source: (Atkins 1990, p. 750).

4.1.12 Activity Coefficient of 0.1 Molar Potassium Chloride

The activity coefficient of 0.1 molar potassium chloride is 0.77.

Source: (Weast 1981, p. D-146).

4.1.13 Diffusion Coefficient of Potassium Chloride

The diffusion coefficient of potassium chloride in solution is 1.844*10⁻⁵ cm²/sec.

Source: (Weast 1981, p. F-53).

4.1.14 Porosity range

The accepted minimum porosity of unconsolidated sand is 30 percent (Bear 1972, p. 46). While it is conceivable that poorly sorted sand may have a lower porosity, this value is considered the

lower bound for most samples. The maximum porosity for uniform spherical particles approaches 50 percent (Bear 1972, p. 46). The range of porosity used in this model is between 30 percent and 50 percent.

4.1.15 Effect of Temperature on Diffusion

The diffusivity (D) is proportional to temperature (T, in Kelvin) and inversely proportional to viscosity (η) (i.e., $D \propto T / \eta$).

Source: (Cussler 1997, p. 114).

It follows that if diffusivity (D_0) is known at some [ambient] temperature (T_0), the diffusivity (D) at some [elevated] temperature (T) can be found by:

$$D = D_0 \cdot \frac{\left(\frac{T}{T_0} \right)}{\left(\frac{\eta}{\eta_0} \right)} \quad (\text{Eq. 13})$$

Substituting viscosity (Equation 12) for η and η_0 [using $(b * a^x) / (b * a^y) = a^{x-y}$]:

$$D = D_0 \cdot \frac{\left(\frac{T + 273}{T_0 + 273} \right)}{10^{\left[\frac{1.3272(20-T) - 0.001053(T-20)^2}{T+105} - \frac{1.3272(20-T_0) - 0.001053(T_0-20)^2}{T_0+105} \right]}} \quad (\text{Eq. 14})$$

where:

- D -Adjusted diffusivity, in cm²/sec, at temperature T, in degrees Celsius
- D₀ -Diffusivity, in cm²/sec, at temperature T₀, in degrees Celsius

4.2 CRITERIA

No criteria, as defined in AP-3.10Q, were used in the preparation of this document.

4.3 CODES AND STANDARDS

No codes or standards, as defined in AP-3.10Q, were used in the preparation of this document.

5. ASSUMPTIONS

No assumptions were used in the preparation of this model, this section is therefore not applicable.

6. MODEL

A model for estimating the diffusivity of electrolytes in saturated and unsaturated porous material is developed in Section 6.2. The model has two parts: first, a model for estimating the conductivity of a material is presented in Section 6.1. The inputs into this model are empirical, and accepted data for clean sand is given as an example. This model predicts the conductivity of a material as a function of saturation.

The second part of the model is developed in Section 6.2 and yields a diffusion coefficient based on conductivity (found through direct measurement or through the method in Section 6.1). An additional portion of the model is developed in Section 6.3, and allows the adjustment of diffusion coefficients as a function of temperature. The effects of water composition are conservatively bounded in Section 6.4.

The model is validated by comparison with a collection of measured diffusion coefficients found using traditional techniques. Model validation criteria are developed in Section 6.5.1. Model validation data is developed in Section 6.5.2 and presented in Table 1 and Figure 1.

6.1 RESISTIVITY OF PARTIALLY SATURATED MATERIAL

Archie's law is presented as an estimate of the conductivity of a material based on saturation, resistance of the saturating solution, and porosity. Combining Equation 1 and Equation 4 yields an equation for conductivity as a function of porosity, saturation, and the conductivity of the saturating fluid.

Equation 1:
$$R_{\text{sat}} = R_{\text{water}} * \Phi^{-m}$$

Equation 4:
$$R = R_{\text{sat}} * S_w^{-n}$$

combining equations:
$$R = R_{\text{water}} \Phi^{-m} S_w^{-n}$$

converting to conductivity:
$$C = [R_{\text{water}} \Phi^{-m} S_w^{-n}]^{-1}$$

simplifying:
$$C = C_{\text{water}} \Phi^m S_w^n \quad (\text{Eq. 15})$$

where:

- C - Conductivity of partially saturated material
- C_{water} - Conductivity of water in the pore structure
- Φ - Fractional porosity. Parametric range between 0.30 and 0.50
- S_w - Saturation, fraction of pore volume containing water
- m - Empirical cementation factor
- n - Empirical saturation exponent

The calculated conductivity of sand partially saturated with 0.1 molar potassium chloride is shown for ranges of porosity and saturation in Table 2 and Figure 2.

6.2 DIFFUSIVITY AS A FUNCTION OF CONDUCTIVITY

Traditional steady state measurements of diffusivity in unsaturated media would require inordinate amounts of time to collect. Maintaining boundary conditions over extended time periods is difficult. One indirect method of determining diffusion coefficients at low water content is to use conductivity measurements to calculate diffusion coefficients. The analogy is between the driving forces acting on an ion. In electrical conductivity measurements, the driving force acting on the ions is electrical potential gradient. In diffusion, the driving force acting on the ions is the concentration gradient. These two forces are related through the Nernst-Einstein equation.

Conductance (Equation 16) is found by combining equations 7, 9, 10, and 11:

$$\text{Equation 7:} \quad D_* = 8.931 \times 10^{-10} T \left(\frac{\Lambda_o}{2} \right)$$

$$\text{Equation 9:} \quad \lambda = \kappa / c$$

$$\text{Equation 10:} \quad \kappa = G * \Theta$$

$$\text{Equation 11:} \quad c = a * M$$

$$\text{Combining Equations 9, 10, and 11: } \lambda = (G * \Theta) / (a * M (1L/1000cm^3)) \quad (\text{Eq. 16})$$

Diffusivity is found by combining Equations 7 and 16 (with $\Lambda_o = \lambda$):

$$D = 8.931 \cdot 10^{-10} \cdot T \cdot \left(\frac{G \cdot \Theta \cdot 10^3}{2 \cdot a \cdot M} \right) \quad (\text{Eq. 17})$$

where:

- D_* -Diffusivity of molecule (ionic pair) at infinite dilution, in $cm^2 \text{ sec}^{-1}$
- D -Diffusivity of molecule (ionic pair) in concentrated solution, in $cm^2 \text{ sec}^{-1}$
- λ -Conductance, in $S \text{ cm}^2 \text{ mol}^{-1}$. Adjusted for concentration effects.
- κ -Conductivity, in $S \text{ cm}^{-1}$
- c -Corrected concentration, in mol/L
- G -Measured conductance, in S
- Θ -Cell constant, in cm^{-1}
- a -Activity coefficient, dimensionless
- M -Concentration, in mol/L
- T -Temperature, in K
- Λ_o -Electrolyte conductance at infinite dilution, in $S/\text{equivalent}$

Using the conductivity calculated from Equation 15, diffusivities are calculated in Table 2 and graphed in Figure 3.

Equation 15 is modified to show the diffusivity is found as a function of conductivity:

$$D = 8.931^{-10} \cdot T \cdot \left(\frac{C \cdot 10^3}{2 \cdot a \cdot M} \right) \quad (\text{Eq. 18})$$

simplifying $D = 5.799^{-6} \cdot T \cdot C \quad (\text{Eq. 19})$

simplifying: $D = 1.728 \cdot 10^{-3} C \quad (\text{Eq. 20})$

Equation 15 substitution $D = 1.728 \cdot 10^{-3} \cdot C_{\text{water}} \Phi^m S_w^n \quad (\text{Eq. 21})$

Simplifying: $D = 2.222 \cdot 10^{-5} \Phi^m S_w^n \quad (\text{Eq. 22})$

where:

- D -Diffusivity of 0.1 molar potassium chloride, in cm^2/sec
- f -Activity coefficient, dimensionless. $f = 0.77$ (4.1.12)
- M -Concentration, in mol/L. In this example $M = 0.1 \text{ mol/L}$
- T -Temperature, in K. In this example $T = 298 \text{ K}$ (25 °C)
- C -Conductivity of sample, in S/cm. Equation 15 can be used to find conductivity as a function of porosity and saturation.
- C_{water} -Conductivity of water in the pore structure, in S/cm. For 0.1 molar potassium chloride $C_{\text{water}} = 0.012856$ (4.1.11)
- Φ -Porosity
- S_w -Fractional saturation
- m -cementation factor. For sand $m = 1.3$ (4.1.2)
- n -saturation exponent. For sand $n = 2$ (4.1.4)

6.3 TEMPERATURE EFFECTS ON CONDUCTIVITY AND DIFFUSION

The diffusivity of ions in solution is proportional to temperature and inversely proportional to viscosity (4.1.15).

Equation 14:

$$D = D_0 \cdot \frac{\left(\frac{T + 273}{T_0 + 273} \right)}{10^{\left[\frac{1.3272(20 - T_c) - 0.001053(T_c - 20)^2}{T_c + 105} - \frac{1.3272(20 - T_{co}) - 0.001053(T_{co} - 20)^2}{T_{co} + 105} \right]}}$$

Equation 17:

$$D = 8.931 \cdot 10^{-10} \cdot T_0 \cdot \left(\frac{G \cdot \Theta \cdot 10^3}{2 \cdot a \cdot M} \right)$$

for $T_{co} = 25$ C, the viscosity exponent is:

$$\frac{1.3272 \cdot (20 - T_{co}) - 0.001053 \cdot (T_{co} - 20)^2}{T_{co} + 105} = -0.051 \quad (\text{Eq. 23})$$

Substituting Equation 17 and Equation 23 into Equation 14 and converting to Kelvin (T_0 cancels out of the numerator):

$$D = \frac{\left(8.931 \cdot 10^{-10} \cdot T \cdot \left(\frac{G \cdot \Theta \cdot 10^3}{2 \cdot a \cdot M} \right) \right)}{10^{\left[\frac{1.3272 \cdot (20 - (T - 273)) - 0.001053 \cdot ((T - 273) - 20)^2}{(T - 273) + 105} + 0.051 \right]}}$$

simplifying:

$$D = \frac{\left(8.931 \cdot 10^{-10} \cdot T \cdot \left(\frac{G \cdot \Theta \cdot 10^3}{2 \cdot a \cdot M} \right) \right)}{10^{\left[\frac{1.3272 \cdot (293 - T) - 0.001053 \cdot (T - 293)^2}{T - 168} + 0.051 \right]}} \quad (\text{Eq. 24})$$

For 0.1 molar potassium chloride with conductance measured at temperature T_0 , in Kelvin:

Equation 19:

$$D_0 = 5.799^{-6} \cdot T_0 \cdot C$$

Substituting Equation 19 and Equation 23 into Equation 14 and converting to Kelvin:

$$D = \frac{(5.799 \cdot 10^{-6} \cdot T \cdot C)}{10^{\left[\frac{-1.3272 \cdot (T-293) - 0.001053 \cdot (T-293)^2}{T-168} + 0.051 \right]}} \quad (\text{Eq. 25})$$

Substituting Equation 15 for C:

$$D = \frac{(5.799 \cdot 10^{-6} \cdot T \cdot (C_{\text{water}} \cdot \Phi^m \cdot S_w^n))}{10^{\left[\frac{-1.3272 \cdot (T-293) - 0.001053 \cdot (T-293)^2}{T-168} + 0.051 \right]}} \quad (\text{Eq. 26})$$

For sand partially saturated with 0.1 molar potassium chloride:

$$D = \frac{(7.455 \cdot 10^{-8} \cdot T \cdot (\Phi^{1.3} \cdot S_w^2))}{10^{\left[\frac{-1.3272 \cdot (T-293) - 0.001053 \cdot (T-293)^2}{T-168} + 0.051 \right]}} \quad (\text{Eq. 27})$$

where:

- D - Diffusivity of 0.1 molar potassium chloride at 25 °C, in cm²/sec
- T - Temperature, in K
- C - Conductivity of sample, in S/cm
- C_{water} - Conductivity of water in the pore structure, in S/cm. For 0.1 molar potassium chloride C_{water} = 0.012856 (4.1.11)
- Φ - Fractional porosity
- S_w - Fractional saturation
- m - cementation factor. For sand m=1.3 (4.1.2)
- n - saturation exponent. For sand n=2 (4.1.4)

Using Equation 27, diffusion coefficients are calculated in Table 2 as a function of temperature. These data are also presented in Figure 4.

6.4 EFFECTS OF WATER COMPOSITION ON DIFFUSION AND CONDUCTION

The activity coefficient of an ion in a single salt solution is generally higher than the activity coefficient of an ion in solution with many other ions. This statement is corroborated by Stumm and Morgan (1981, p. 411), where activity coefficients in single salt solutions are compared with activity coefficients measured in seawater. The model does not account for background electrolyte effects, which is conservative (bounding).

6.5 MODEL VALIDATION

The invert diffusion properties model is validated in Section 6.5.2 by comparing the validation data with the validation criteria presented in Section 6.5.1.

6.5.1 Validation Criteria

The model has two parts, conductivity prediction and diffusion prediction. The conductivity portion of the model is accepted fact. The prediction of conductivity of materials other than those presented in Section 6.2 (sand) requires the collection of the empirical cementation and saturation exponents from accepted or qualified sources.

The second portion of the model, prediction of diffusion coefficients, is considered validated for cases where the predictions are conservative when compared to diffusion coefficients collected using traditional, non-electrical, techniques.

6.5.2 Validation Results

A collection of diffusion coefficients is published in Lim et al. (1998, p. 813). The graph in this reference plots the diffusion coefficient, normalized with respect to the diffusion coefficient in bulk solution, against volumetric water content. The model developed in Section 6.2 is normalized and plotted against volumetric water content. The normalized diffusion coefficient (D_n) is:

$$D_n = \phi^{1.3} S_w^2$$

Volumetric water content is the product of saturation and porosity. Table 1 shows the normalized diffusivity and volumetric water content for sand with 30 percent, 40 percent, and 50 percent porosity (Section 4.1.14). These data are also presented in Figure 1.

Comparing Figure 1 with the diffusion coefficients published in Lim et al. (1998, p. 813) illustrates the conservative nature of the model. Excluding Conca's results in Lim et al. (1998, Figure 1), which were calculated from conductivity, the predicted diffusion coefficients are larger than reported experimental values for every instance of moderate to low water contents. The model may be less conservative for near saturated conditions, at which point the diffusive barrier is ineffective. Even at near saturated conditions, the model agrees with the actual diffusion coefficients cited.

Table 1. Normalized Diffusivity as a Function of Saturation and Water Content.

S_w	V_{30}	D_{30}	V_{40}	D_{40}	V_{50}	D_{50}
Porosity:	0.3		0.4		0.5	
0.1%	0.03%	2.1E-07	0.04%	3.0E-07	0.05%	4.1E-07
0.5%	0.15%	5.2E-06	0.20%	7.6E-06	0.25%	1.0E-05
1%	0.3%	2.1E-05	0.4%	3.0E-05	0.5%	4.1E-05
5%	1.5%	5.2E-04	2.0%	7.6E-04	2.5%	1.0E-03
10%	3%	2.1E-03	4%	3.0E-03	5%	4.1E-03
20%	6%	8.4E-03	8%	1.2E-02	10%	1.6E-02
30%	9%	1.9E-02	12%	2.7E-02	15%	3.7E-02
50%	15%	5.2E-02	20%	7.6E-02	25%	1.0E-01
60%	18%	7.5E-02	24%	1.1E-01	30%	1.5E-01
70%	21%	1.0E-01	28%	1.5E-01	35%	2.0E-01
80%	24%	1.3E-01	32%	1.9E-01	40%	2.6E-01
90%	27%	1.7E-01	36%	2.5E-01	45%	3.3E-01
100%	30%	2.1E-01	40%	3.0E-01	50%	4.1E-01

Notes:

S_w is percent saturation.

V_{30} , V_{40} , and V_{50} are the volumetric water content of 30%, 40% and 50% porosity sand, respectively.

D_{30} , D_{40} , and D_{50} is the diffusivity of 30%, 40%, and 50% porosity sand, respectively.

V_{30} , V_{40} , and V_{50} are the product of saturation and porosity [=Porosity * Saturation].

D_{30} , D_{40} , and D_{50} were calculated with the equation developed in 6.5.2. $[(\text{Porosity})^{1.3} * (\text{Saturation})^2]$

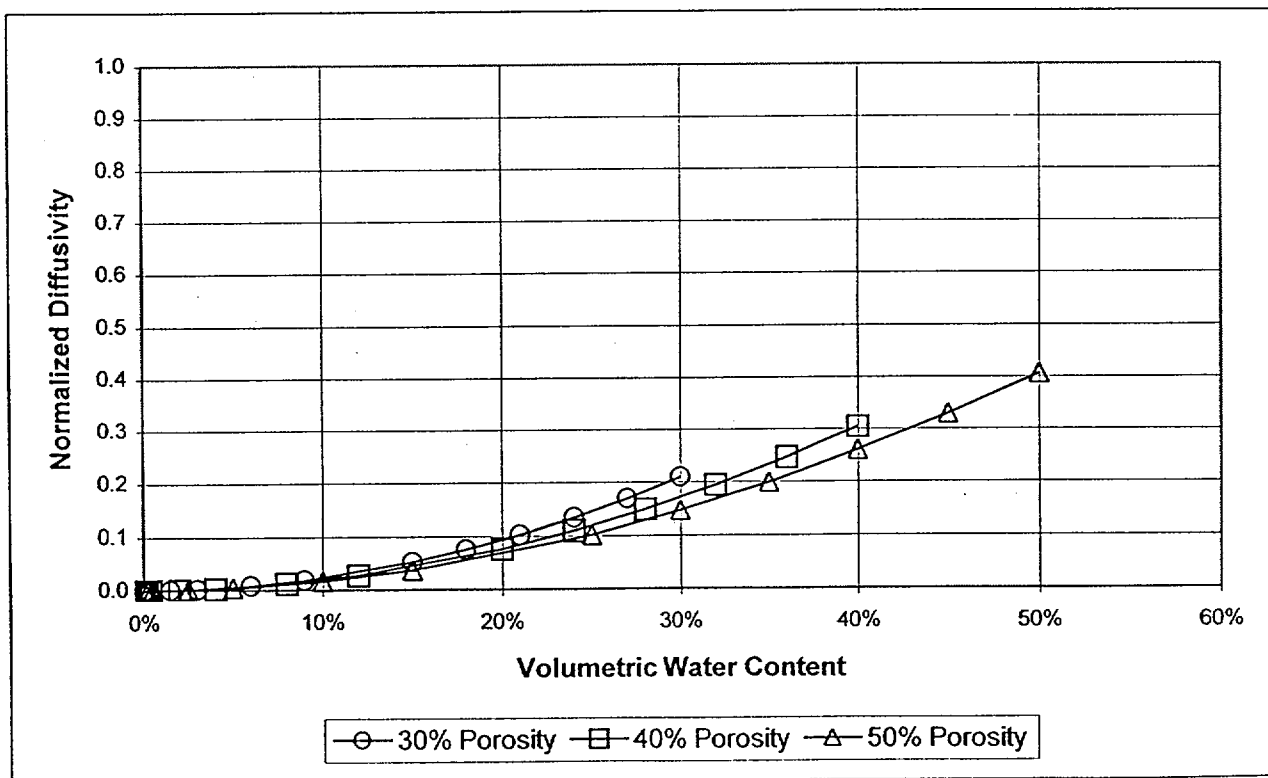


Figure 1. Normalized Diffusivity vs. Water Content.

7. CONCLUSIONS

The diffusivity of a given material can be predicted from conductivity measurements or basic material properties, including two empirical constants. The models in this document were validated in Section 6.5.2.

Equation 15

$$C = C_{\text{water}} * \Phi^m * S_w^n$$

where:

- C - Conductivity of the material
- C_{water} - Conductivity of the saturating material
- Φ - Porosity. Parametric range between 30% and 50%
- m - Empirical cementation factor
- n - Empirical saturation exponent

The diffusivity can be found from conductivity through the following :

Equation 17:

$$D = 8.931 \cdot 10^{-10} \cdot T \cdot \left(\frac{G \cdot \Theta \cdot 10^3}{2 \cdot a \cdot M} \right)$$

where:

- D - Diffusivity, in $\text{cm}^2 \text{sec}^{-1}$
- G - Measured conductance, in S
- Θ - Cell constant, in cm^{-1}
- a - Activity coefficient, dimensionless
- M - Concentration, in mol/L
- T - Temperature, in K

A modification of this model includes a temperature adjustment:

Equation 24:

$$D = \frac{\left(8.931 \cdot 10^{-10} \cdot T \cdot \left(\frac{G \cdot \Theta \cdot 10^3}{2 \cdot a \cdot M} \right) \right)}{10^{\left[\frac{-1.3272(T-293) - 0.001053(T-293)^2}{T-168} + 0.051 \right]}}$$

where:

- G - Measured conductance, in S
- Θ - Cell constant, in cm⁻¹
- a - Activity coefficient, dimensionless
- M - Concentration, in mol/L
- T - Temperature, in K

7.1 RESULTS

Conductivity and diffusivity are presented in Table 2. Figure 2 is a log-log plot of conductivity as a function of water content. Figure 3 is a log-log plot of diffusivity as a function of water content. Figure 4 is a log-log plot of diffusivity as a function of temperature for a material at a porosity of 40%.

Table 2. Diffusion Coefficients and Conductivity

Sw	Vw	Vw	Vw	C	C	C	D	D	D	Dt	Dt	Dt	Dt
Temperature, in degrees Celsius:										20	50	70	90
Porosity:	30%	40%	50%	30%	40%	50%	30%	40%	50%	40%	40%	40%	40%
0.1%	0.03%	0.04%	0.05%	2.7E-09	3.9E-09	5.2E-09	4.6E-12	6.8E-12	9.0E-12	5.9E-12	1.2E-11	1.7E-11	2.3E-11
0.3%	0.09%	0.12%	0.15%	2.4E-08	3.5E-08	4.7E-08	4.2E-11	6.1E-11	8.1E-11	5.3E-11	1.1E-10	1.5E-10	2.1E-10
0.5%	0.15%	0.20%	0.25%	6.7E-08	9.8E-08	1.3E-07	1.2E-10	1.7E-10	2.3E-10	1.5E-10	3.0E-10	4.3E-10	5.8E-10
0.7%	0.21%	0.28%	0.35%	1.3E-07	1.9E-07	2.6E-07	2.3E-10	3.3E-10	4.4E-10	2.9E-10	5.8E-10	8.4E-10	1.1E-09
1%	0.3%	0.4%	0.5%	2.7E-07	3.9E-07	5.2E-07	4.6E-10	6.8E-10	9.0E-10	5.9E-10	1.2E-09	1.7E-09	2.3E-09
3%	0.9%	1.2%	1.5%	2.4E-06	3.5E-06	4.7E-06	4.2E-09	6.1E-09	8.1E-09	5.3E-09	1.1E-08	1.5E-08	2.1E-08
5%	1.5%	2.0%	2.5%	6.7E-06	9.8E-06	1.3E-05	1.2E-08	1.7E-08	2.3E-08	1.5E-08	3.0E-08	4.3E-08	5.8E-08
7%	2.1%	2.8%	3.5%	1.3E-05	1.9E-05	2.6E-05	2.3E-08	3.3E-08	4.4E-08	2.9E-08	5.8E-08	8.4E-08	1.1E-07
10%	3%	4%	5%	2.7E-05	3.9E-05	5.2E-05	4.6E-08	6.8E-08	9.0E-08	5.9E-08	1.2E-07	1.7E-07	2.3E-07
13%	4%	5%	7%	4.5E-05	6.6E-05	8.8E-05	7.9E-08	1.1E-07	1.5E-07	1.0E-07	2.0E-07	2.9E-07	3.9E-07
15%	5%	6%	8%	6.0E-05	8.8E-05	1.2E-04	1.0E-07	1.5E-07	2.0E-07	1.3E-07	2.7E-07	3.9E-07	5.2E-07
17%	5%	7%	9%	7.8E-05	1.1E-04	1.5E-04	1.3E-07	2.0E-07	2.6E-07	1.7E-07	3.4E-07	4.9E-07	6.7E-07
20%	6%	8%	10%	1.1E-04	1.6E-04	2.1E-04	1.9E-07	2.7E-07	3.6E-07	2.4E-07	4.8E-07	6.9E-07	9.3E-07
30%	9%	12%	15%	2.4E-04	3.5E-04	4.7E-04	4.2E-07	6.1E-07	8.1E-07	5.3E-07	1.1E-06	1.5E-06	2.1E-06
40%	12%	16%	20%	4.3E-04	6.3E-04	8.4E-04	7.4E-07	1.1E-06	1.4E-06	9.4E-07	1.9E-06	2.7E-06	3.7E-06
50%	15%	20%	25%	6.7E-04	9.8E-04	1.3E-03	1.2E-06	1.7E-06	2.3E-06	1.5E-06	3.0E-06	4.3E-06	5.8E-06
70%	21%	28%	35%	1.3E-03	1.9E-03	2.6E-03	2.3E-06	3.3E-06	4.4E-06	2.9E-06	5.8E-06	8.4E-06	1.1E-05
90%	27%	36%	45%	2.2E-03	3.2E-03	4.2E-03	3.8E-06	5.5E-06	7.3E-06	4.8E-06	9.7E-06	1.4E-05	1.9E-05

Notes:

(Sw) Saturation (Sw) is a parametric value ranging between 0.1% and 100%

(Vw) Volumetric Water Content (Vw) is the product of porosity and saturation.

(C) = $(0.012856 * (\text{Porosity})^{1.3} * (\text{Saturation})^2)$. Source: Equation 15 with $C_{\text{water}} = 0.012856$ (4.1.11).(D) = $2.222 * 10^{-5} * ((\text{Porosity})^{1.3} * (\text{Saturation})^2)$. Source: Equation 22.(Dt) = $(7.455 * 10^{-5} * (\text{Temp. in K}) * (\text{porosity})^{1.3} * (\text{Sw})^2) / [10^{(-1.3172 * (20 - \text{Temp in } ^\circ\text{C})) - 0.001053 * ((\text{Temp in } ^\circ\text{C} - 20)^2) / (\text{Temp in } ^\circ\text{C} + 105) + 0.051}]$

Source: Equation 27.

While saturation (Sw) and volumetric water content (Vw) are displayed as percentages, the fractional values are used in calculations.

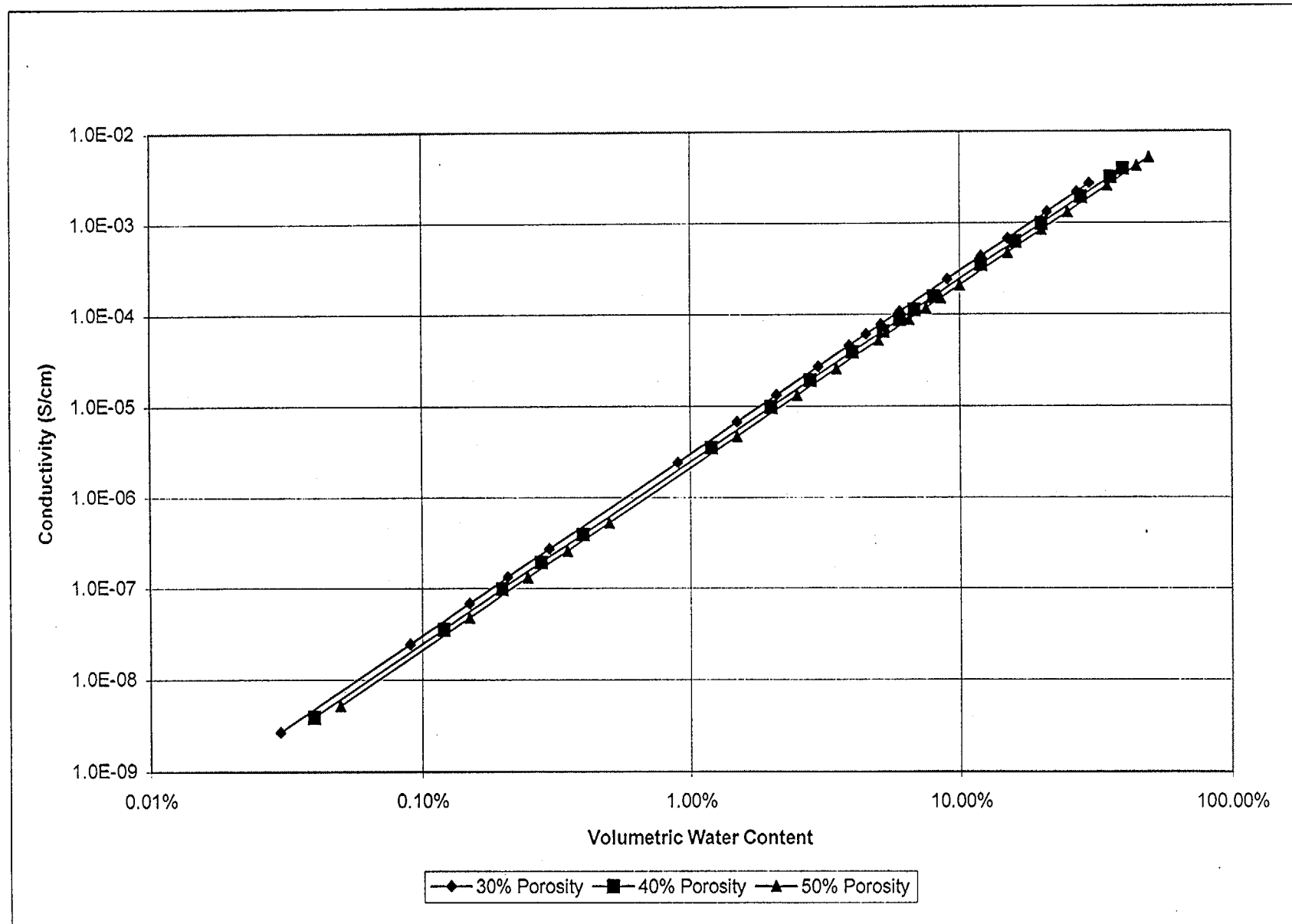


Figure 2. Log Plot of Conductivity vs. Water Content

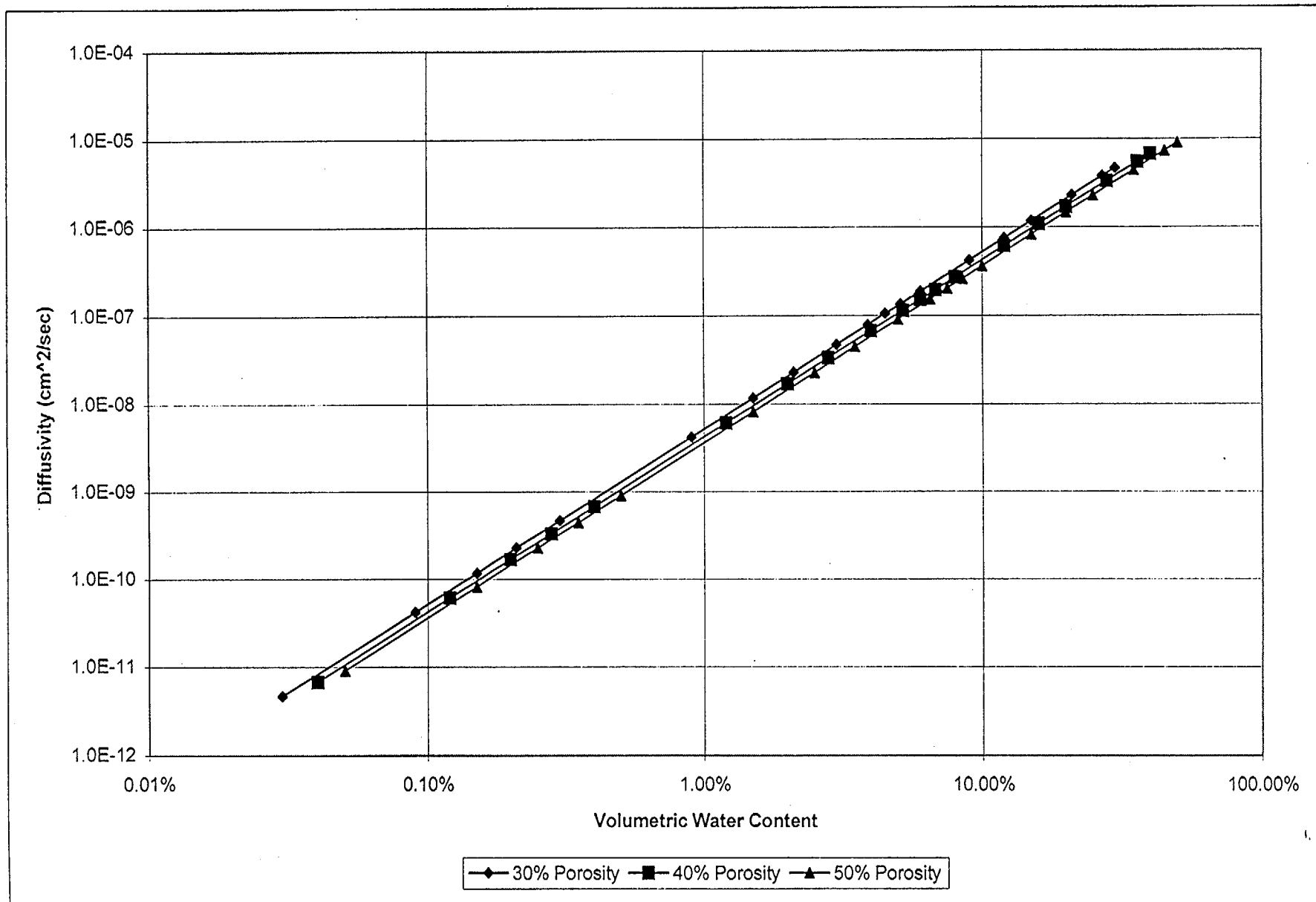


Figure 3. Log Plot of Diffusivity vs. Water Content

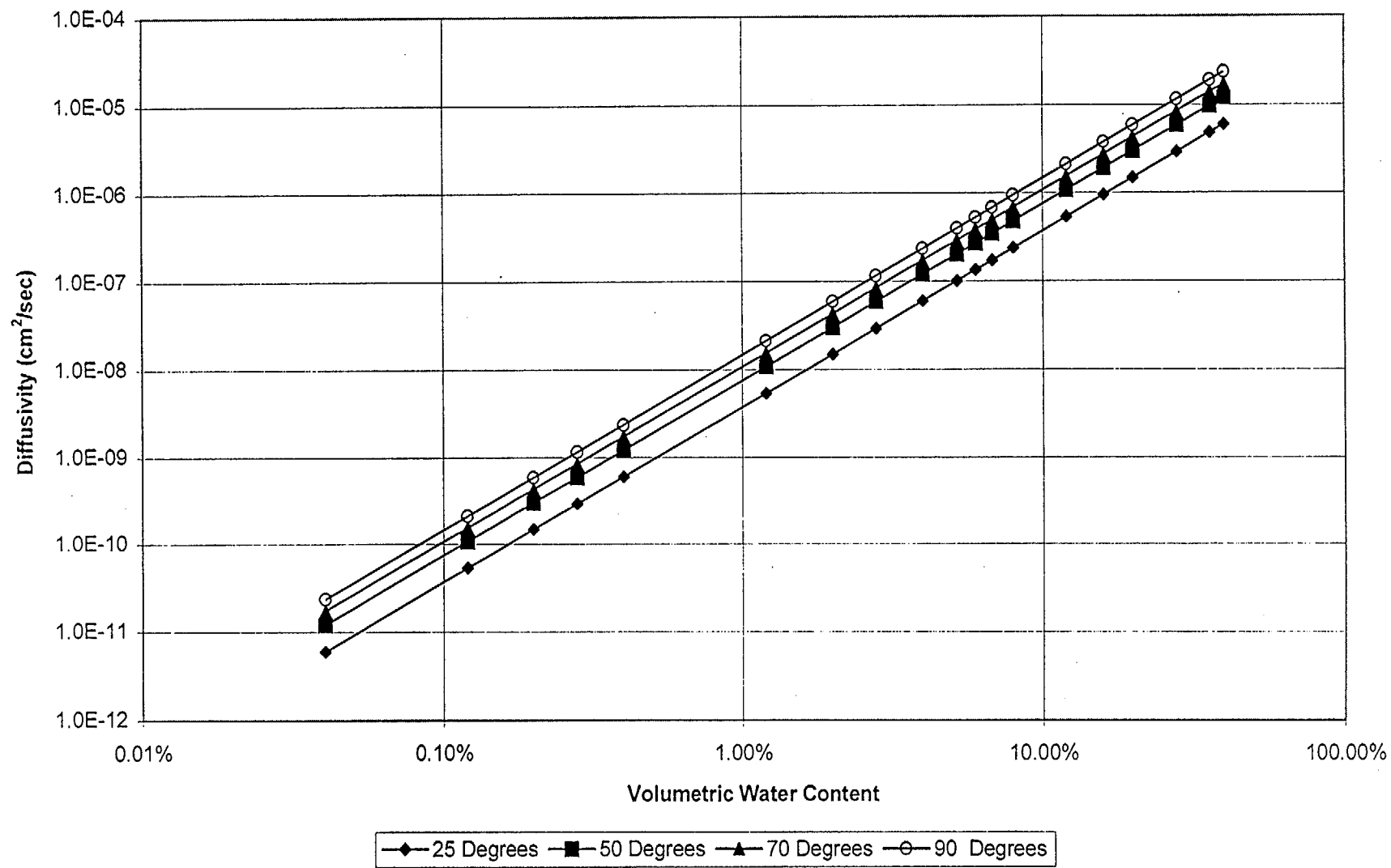


Figure 4. Log Plot Temperature Dependent Diffusivity vs. Water Content at 40% Porosity

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AP-3.4Q, Rev 01. *Level 3 Change Control*. Washington, D.C.: DOE OCRWM. ACC: MOL.19990923.0230.

AP-3.10Q, Rev 01. *Analyses and Models*. Washington, D.C.: DOE OCRWM. ACC: MOL.19990702.0314.

AP-3.15Q, Rev 00, ICN 1. *Managing Technical Product Inputs*. Washington, D.C.: DOE OCRWM. ACC: MOL.19990831.0079.

AP-SIII.3Q, Rev 00. *Submittal and Incorporation of Data to the Technical Data Management System*. Washington, D.C.: DOE OCRWM. ACC: MOL.19990702.0319.

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QAP-2-3, Rev 10. *Classification of Permanent Items*. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990316.0006.

9. ATTACHMENTS

	Pages
Attachment I: Document Input Reference Sheets.....	I-1 - I-9
Attachment II: Mathematical Proof	I-1 - I-2

ATTACHMENT I
DOCUMENT INPUT REFERENCE SHEETS

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

1. Document Identifier No./Rev.: ANL-EBS-MD-000031 REV 00			Change: --		Title: Invert Diffusion Properties Model				
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	Atkins, P.W. 1990. <i>Physical Chemistry, 4th Edition</i> . New York, New York: W. H. Freeman and Company. TIC: 245483.	Cover	N/A (Est. fact)	entire	Gas constant	N/A	N/A	N/A	N/A
1		Cover	N/A (Est. fact)	entire	Faraday's constant				
		p. 750	N/A (Equation)	4.1.6, 6.2	Molar conductivity equation				
		p. 750	N/A (Equation)	4.1.7, 6.2	Conductance equation				
		p. 750	N/A (Equation)	4.1.7, 4.1.11, 6.2	Conductivity is the inverse of resistivity. Conductance is the inverse of resistance.				
2	Bear, J. 1972. <i>Dynamics of Fluids in Porous Media</i> . New York, New York: American Elsevier Publishing Company, Inc. TIC: 217568.	p. 113	N/A-Corroborative	4.1.1	Equation: formation factor (F) from resistance.	N/A	N/A	N/A	N/A
		p. 116	N/A-Corroborative	4.1.1	Equation: F from porosity, cementation.				
		p. 116	N/A-Corroborative	entire	Cementation factor for sand.				
		p. 116	N/A-Corroborative	4.1.3, 6.1	Archies equation for resistivity of unsaturated media.				
		p. 116	N/A-Corroborative	entire	Saturation exponent.				
		p. 46	N/A (Reference)	4.1.14	Range of porosity.				

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2. Technical Product Input Source Title and Identifier(s) with Version	Unqual.						From Uncontrolled Source	Un-confirmed	
3	CRWMS M&O 1999a. <i>Classification of the Preliminary MGDS Repository Design.</i> B00000000-01717-0200-00134 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19981103.0546.	IV-1	N/A (Reference)	2	Classification of systems	N/A	N/A	N/A	N/A
4	CRWMS M&O 1999b. <i>Development Plan for Invert Diffusion Properties Model.</i> TDP- EBS-MD-000016 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990813.0391.	All	N/A (Reference)	2	Development plan of document	N/A	N/A	N/A	N/A
5	CRWMS M&O 1999c. <i>Activity Evaluation for Engineered Barrier System Performance Modeling (WP# 12012383MX).</i> Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990719.0317.	All	N/A (Reference)	2	Activity Evaluation	N/A	N/A	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	
6	Cussler, E.L. 1997. <i>Diffusion: Mass Transfer in Fluid Systems</i> . 2 nd Edition. New York, New York: Cambridge University Press. TIC: 241150.	p. 114	N/A (Reference)	4.1.15, 6.3	Effect of temperature and viscosity on the diffusion coefficient.	N/A	N/A	N/A	N/A
7	DOE (U.S. Department of Energy) 1998a. <i>Quality Assurance Requirements and Description (QARD)</i> . DOE/RW-0333P REV 8. Washington, D.C.: DOE Office of Civilian Radioactive Waste Management. ACC: MOL.19980601.0022.	All	N/A (Reference)	2	Requirements Document	N/A	N/A	N/A	N/A
8	DOE 1998b. <i>Q-List</i> . YMP/90-55Q REV 5. Las Vegas, Nevada: OCRWM. ACC: MOL.19980513.0132.	p. II-9	N/A (Reference)	2	Q-List Requirements	N/A	N/A	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	
9	Keller, G.V. and Frischknecht, F. C. 1966. <i>Electrical Methods in Geophysical Prospecting</i> . New York, New York: Pergamon Press. TIC: 230941.	p. 21 p. 28 p. 28	N/A (Equation) N/A (Equation) N/A-Corroborative	4.1.1, 6.1 4.1.3, 6.2 entire	Archie's law: resistivity of saturated media. Archies law for resistivity of unsaturated media. Saturation exponent for unsaturated sand.	N/A	N/A	N/A	N/A
10	Lim, P.C.; Barbour, S.L.; and Fredlund, D.G. 1998. "The influence of degree of saturation on the coefficient of aqueous diffusion. " <i>Canadian Geotechnical Journal</i> , 35, 811-827. Ottawa, Ontario: NRC Research Press. TIC: 245626.	Pg. 813, Figure 1.	N/A-Corroborate with model results for validation purposes.	6.5	Diffusion coefficients found using traditional techniques.	N/A	N/A	N/A	N/A
11	Perry, R.H. and Chilton, C.H. 1973. <i>Chemical Engineers' Handbook, 5th Edition</i> . New York, New York: McGraw-Hill Book Company. TIC: 242591.	3-235 3-235	N/A (Established facts from engineering handbook)	4.1.5 4.1.5	Diffusivity found using conductance Electrolyte conductance is the sum of ionic conductances	N/A N/A	N/A N/A	N/A N/A	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	
12	Pirson, S.J. 1963. <i>Handbook of Well Log Analysis: For Oil and Gas Formation Evaluation</i> . Englewood Cliffs, New Jersey: Prentice-Hall, Inc. TIC: 245393.	p. 22 p. 23 p. 24 p. 24 p. 24	N/A (Established facts from engineering handbook)	4.1.1 4.1.1 entire 4.1.3, 6.1 entire	Equation: formation factor (F) from resistance. Equation: F from porosity, cementation. Cementation factor for sand. Archies equation for resistivity of unsaturated media. Saturation exponent.	N/A	N/A	N/A	N/A
13	Robinson, R.A. and Stokes, R.H. 1965. <i>Electrolyte Solutions: The Measurement and Interpretation of Conductance, Chemical Potential and Diffusion in Solutions of Simple Electrolytes</i> . London, England: Butterworths Publications Limited. TIC: 242575.	p. 462	N/A (Reference)	4.1.11, 6.1	Conductivity of 0.1 molar potassium chloride.	N/A	N/A	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	
14	Stumm, W. and Morgan, J. J. 1981. <i>Aquatic Chemistry: An Introduction Emphasizing Chemical Equilibria in Natural Waters. 2nd Edition.</i> New York, New York: John Wiley & Sons, Inc. TIC: 208448.	p. 411	N/A (Reference)	6.4	The activity coefficient of an ion in a single salt solution is higher than the activity coefficient of an ion in solution with many other ions.	N/A	N/A	N/A	N/A
15	Weast, R.C., ed. 1981. <i>CRC Handbook of Chemistry and Physics: A Ready-Reference Book of Chemical and Physical Data, 62nd Edition.</i> Boca Raton, Florida: CRC Press. TIC: 240722	p. F-79 p. F-42 p. F-42 p. D-146 p. F-53	N/A (Established facts from scientific handbook)	4.1.8, 6.2 4.1.9, 6.3 4.1.10, 6.3 4.1.12, 6.2 4.1.13, 6.5.2	Activity effect of concentration. Viscosity of water at 20 degrees Celsius. Viscosity of water as a function of temperature. Activity coefficient of 0.1 molar potassium chloride. Diffusion coefficient of 0.1 molar potassium chloride.	N/A	N/A	N/A	N/A

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DOCUMENT INPUT REFERENCE SHEET

1. Document Identifier No./Rev.: ANL-EBS-MD-000031 REV 00			Change: --		Title: Invert Diffusion Properties Model				
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	
16	AP-2.13Q, REV 00. <i>Technical Product Development Planning</i> . Washington, D.C.: DOE OCRWM. ACC: MOL.19990701.0617.	All	N/A (Reference)	2	Procedure	N/A	N/A	N/A	N/A
17	AP-3.4Q, REV 01. <i>Level 3 Change Control</i> . Washington, D.C.: DOE OCRWM. ACC: MOL.19990701.0624.	All	N/A (Reference)	2	Procedure	N/A	N/A	N/A	N/A
18	AP-3.10Q, REV 01. <i>Analyses and Models</i> . Washington, D.C.: DOE OCRWM. ACC: MOL.19990702.0314.	All	N/A (Reference)	2	Procedure	N/A	N/A	N/A	N/A
19	AP-3.15Q, REV 00, ICN 1. <i>Managing Technical Product Inputs</i> . Washington, D.C.: DOE OCRWM. ACC: MOL.19990831.0079.	All	N/A (Reference)	2	Procedure	N/A	N/A	N/A	N/A
20	AP-SIII.3Q, REV 00. <i>Submittal and Incorporation of Data to the Technical Data Management System</i> . Washington, D.C.: DOE OCRWM. ACC: MOL.19990702.0319.	All	N/A (Reference)	2	Procedure	N/A	N/A	N/A	N/A

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DOCUMENT INPUT REFERENCE SHEET**

1. Document Identifier No./Rev.: ANL-EBS-MD-000031 REV 00			Change: --		Title: Invert Diffusion Properties Model				
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
21	QAP-2-0, REV 05. <i>Conduct of Activities</i> . Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980826.0209.	All	N/A (Reference)	2	Procedure	N/A	N/A	N/A	N/A
22	QAP-2-3, REV 10. <i>Classification of Permanent Items</i> . Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990316.0006.	All	N/A (Reference)	2	Procedure	N/A	N/A	N/A	N/A

**ATTACHMENT II
MATHEMATICAL PROOF**

The square of the average of two numbers is always greater than their product. Consider two non-negative numbers A and B:

$$\begin{aligned}
 \left[\frac{(A+B)}{2} \right]^2 & \geq (AB) \\
 \left[\frac{(A+B)^2}{4} \right] & \geq (AB) \\
 [A^2 + 2AB + B^2] & \geq (4AB) \\
 [A^2 + B^2] & \geq (2AB) \\
 [A^2 + B^2 - (2AB)] & \geq 0
 \end{aligned}
 \tag{Eq. II-1}$$

From basic calculus, the minimum of the expression is found. Taking the first derivative and setting equal to zero will show where the maximum or minimum of the equation occurs. The derivative of Equation II-1 with respect to A is:

$$\begin{aligned}
 D_A [A^2 + B^2 - (2AB)] &= 0 \\
 2A - 2B &= 0 \\
 A &= B
 \end{aligned}$$

To determine whether this point is a maximum or a minimum take the second derivative of Equation II-1 is:

$$D_A (2A - 2B) = 2$$

The positive sign of the second derivative at the point A=B indicates that the minimum of the expression occurs at the point A=B. Substituting B for A in Equation II-1 yields:

$$\begin{aligned}
 [B^2 + B^2 - (2B \cdot B)] & \geq 0 \\
 2B^2 - 2B^2 & \geq 0 \\
 0 & \geq 0
 \end{aligned}$$

This statement is true, which proves the following inequality (i.e. the square of the average of two unique numbers is always greater than their product):

$$\left[\frac{(A+B)}{2} \right]^2 \geq (AB) \tag{Eq. II-2}$$