

Groundwater Modeling for the WCS Site Model v0.205

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1.0 Background

Groundwater at the Waste Control Specialists (WCS) Andrews Facility is here defined as all water in porous media below the ground surface. The disposal of wastes in the Compact Waste Facility (CWF) and Federal Facility Waste Disposal Facility (FWF) is contained within engineered disposal units entirely within the unsaturated zone (UZ), and the bulk of contaminant transport also occurs in the UZ. The UZ is conceptualized to extend to the top of the 225-ft sandstone, based on a conceptual model developed as part of the original license application (LA) (WCS, 2007) submitted by WCS to the Texas Commission on Environmental Quality (TCEQ). In that conceptualization, water was allowed to slowly flow down through the layers of the cover, waste, and underlying natural claystone and sandstone deposits to the “225”, where it is modeled as traveling laterally to a hypothetical domestic water supply well. For the purposes of this updated model (WCS Site Model v0.205) this conceptual model of groundwater flow is honored, though hydrogeologic investigations have demonstrated that no net flow actually occurs in the waste horizon. Since the flow in the saturated zone (SZ, conceptualized to be the 225-ft sandstone) was linked to the recharge flow into it from the overlying UZ, no flow occurs in the SZ, either. With no advective flow of water, the entire system is diffusion dominated.

2.0 Summary of Parameter Values

A summary of parameter values used in the WCS Site Model v0.205 is provided in Table 1. For distributions, the following notation is used:

- $N(\mu, \sigma, [min, max])$ represents a normal distribution with mean μ and standard deviation σ , and optional truncation at the specified *minimum* and *maximum*,
- $LN(GM, GSD)$ represents a log-normal distribution with geometric mean GM and geometric standard deviation GSD,
- $U(min, max)$ represents a uniform distribution with lower bound min and upper bound max, and
- $Beta(\mu, \sigma, min, max)$ represents a generalized beta distribution with mean μ , standard deviation σ , minimum min, and maximum max.

Note that a number of these distributions are truncated at a minimum value of 0 and a maximum of Large, a very large value defined in the GoldSim model. The truncation at the low end is a matter of physical limits (e.g. precipitation cannot be negative), and in GoldSim’s distribution definitions, if truncations are made, they must be made at both ends, so the very large value is chosen for the upper end. Some distributions are truncated at the low end just above zero, using a very small value, Small.

Table 1. Summary of parameter values and distributions.

Parameter	Distribution	Units	Internal Reference
water phase transport			
Water content exponent for water tortuosity	N(7/3, 0.001)	—	Section 3.3.1
Porosity exponent for water tortuosity	N(2, 0.001)	—	Section 3.3.1
air phase transport			
Thickness of the atmosphere layer	N(2.0, 0.1, Small, Large)	m	Section 4.2.1
Wind speed	N(3.14, 0.1, Small, Large)	m/s	Section 4.2.1
Atmospheric diffusion length	N(0.15, 0.02, Small, Large)	m	Section 4.2.1
radon emanation			
Radon E/P ratio	N(0.2, 0.01, 0, 1)	—	Section 4.3.1
legacy groundwater scenario			
Saturated hydraulic conductivity for 225-ft sandstone	LN(8.87E-9, 1.33)	cm/s	Section 5.0
Well casing diameter	Beta(7.0, 2.1, 1.5, 12.5)	in	Section 5.0

3.0 Unsaturated Zone Water

3.1 Unsaturated Zone Flow Modeling – LLW Cells

Estimates of net infiltration through the column and material water saturation required by the GoldSim model (the WCS Site Model) were made using HYDRUS 2D models of the disposal system developed by INTERA. This flow modeling was performed external to the WCS Site Model, which is developed on the GoldSim modeling platform, and results of the HYDRUS modeling were imported into GoldSim model elements. The WCS Site Model calculates contaminant transport within two 1-D columns, one each for the CWF and the FWF. These columns contain layers of various materials, and contaminant fate and transport is subject to a number of simultaneous processes, including potential advection of groundwater (tied to uniform infiltration through the column), diffusion in water and air phases, biotically-induced transport, and radioactive decay and ingrowth. Infiltration is assumed to uniform throughout the column, matched to the values produced by HYDRUS at the 5-m depth. Saturations in the various layers are also imported from the HYDRUS modeling, and strongly influence local tortuosities which in turn strongly influence effective rates of diffusion in pore water and air.

Details of the HYDRUS unsaturated zone flow models for the LLW disposal units are provided in Appendix 2 of the *Updated Performance Assessment for the Low-Level Waste Facility, Waste Control Specialists LLC, Andrews, Texas* (WCS, 2011). Scenarios 2, 5, and 9 as described in this Appendix were chosen to conduct further sensitivity runs. Scenarios 2 and 5 used current climate and constant head boundary conditions at a 5-meter (m) depth below ground surface (bgs).

Differences between scenarios 2 and 5 were that scenario 2 used as-built material properties for the red bed clay fill and the performance clay and scenario 5 considered naturalized properties for these layers. The material property changes modeled included changes in one of the hydraulic model parameters (van Genuchten's α) for the red bed clay fill, and changes in α and the saturated hydraulic conductivity in the performance clay layer. Scenario 9 considered future climate conditions, naturalized material properties as described for scenario 5, and constant head boundary conditions at 5 m bgs.

Multiple realizations were run for each of the three scenarios. Realizations consisted of variations in precipitation timing for all three scenarios, and also variations in root depth together with leaf area index (LAI) for the current climate scenarios. Three variations in precipitation and potential evapotranspiration were modeled. The first represented the observed climate. The second, a shuffled time series representing the same mean annual precipitation, but having the least number of consecutive wet years. The third was also a shuffled time series but in this case representing the largest number of consecutive wet years.

For each set of climate time series for the current climate there were three different configurations of root depth and leaf area index corresponding to plants with deep roots and a large LAI, mid-range depth roots and a mid-range LAI, and shallow roots and a small LAI. Plant parameters were not varied for the future climate scenario. Steady-state net infiltration and material water saturation inputs from these models were provided by INTERA to Neptune's GoldSim model developers in the Microsoft Excel workbook *Stochastic Infiltration Modeling for WCS PA.xlsx*.

3.2 Unsaturated Zone Flow Modeling – RCRA Cells

Modeling of the RCRA Landfill is incomplete as of the WCS Site Model v0.205. This section is reserved for subsequent versions that will develop and discuss unsaturated zone modeling for the RCRA Landfill, which is different from that of the LLW disposal facilities, due to the nature of the RCRA cover.

3.3 Modeling Diffusion in Unsaturated Porous Media

The WCS Site Model employs a modified version of GoldSim's native diffusive flux links to calculate diffusive fluxes in porous media. The modifications are necessary to account for unsaturated media, since GoldSim assumes that porous media are saturated in its basic implementation of diffusive flux calculations. The standard GoldSim diffusive flux mathematics are covered in Appendix B of the GoldSim User's Guide (GTG, 2011), and the modifications that have been developed by Neptune are discussed in detail in the Neptune document entitled *Modeling Diffusion in GoldSim*, but are also covered briefly here. The modifications that are required in order to properly model diffusion in unsaturated media take two phenomena into consideration: 1) The diffusive area is reduced by the saturation (with respect to air or water, whichever medium is of interest) and 2) the diffusive length is increased to account for tortuosity in the respective medium.

If a porous medium contains only a single fluid phase, the diffusive area between two cells containing that medium is simply the total area times the porosity, since the pores are occupied

by the fluid and the diffusion takes place only in the fluid. In the case of two fluids, such as air and water in unsaturated media, the diffusive area is further reduced, since the area of the fluid of interest across the plane of diffusion is less. If we are interested in diffusion in the water phase, for example, the area of water that intersects the plane is equal to the total area times the water content, which equals the total area times the porosity times the saturation with respect to water. If we are interested in diffusion in the air phase, we use the same construct, substituting air for water. Because the diffusive area is always less, the diffusion in an unsaturated medium will always be less than that in a fully saturated medium.

Diffusion in unsaturated media is also attenuated because of increased tortuosity. In any porous medium, a diffusing solute must travel through pores, following a tortuous path that is always longer than if it were traveling in a straight line. The ratio of the straight line distance to this tortuous path is called the tortuosity. If the porous medium is unsaturated, this path becomes even longer, since the three dimensional shape of the fluid of interest gets even more tortuous. This increases the diffusive length, which is used in calculating the concentration gradient. The gradient in concentration of a solute is what drives diffusion.

3.3.1 Water Phase Tortuosity

Tortuosity is a term used to describe the resistive and retarding influence of pore structure for a variety of transport processes (Clennell, 1997). Definitions of tortuosity are not consistent in the literature and depend on the discipline and the particular transport process of interest. The tortuosity τ for molecular diffusion in porous media can be written as the ratio of effective diffusivity D_{eff} to bulk diffusivity D_{bulk} , often seen in two forms:

$$\tau_1 = \frac{D_{eff}}{D_{bulk}} \quad (1)$$

or alternatively, if exclusion of the measured porosity n is desired (Clennell, 1997), as

$$\tau_1 = \frac{D_{eff}}{n D_{bulk}}. \quad (2)$$

In this definition, consistent with the assumptions of GoldSim's internal calculations, the value of tortuosity varies between 0 and $1/n$, with lower values indicating a longer path for porous medium solute transport via diffusion. For unsaturated systems n is replaced in equation (2) by water content θ_w for water phase diffusion, or by the volumetric air content θ_a , for gaseous phase diffusion. The form shown in equation (1) is found in Freeze and Cherry (1979) and Marsily (1986) while that in equation (2) is used by Hillel (1980) and Koorevaar et al. (1983).

For consistency with GoldSim the second form is used. The equations for diffusive transport in GoldSim explicitly specify the effective porosity (or in the case of unsaturated flow, water content or air filled porosity) as in equation (2). For more information on the diffusive mass flux equations in GoldSim, see Appendix B of the GoldSim User's Guide (GTG, 2011). In the following sections, the equations from the literature have been converted where necessary to be consistent with equation (2) so that they can be directly applied to GoldSim models.

Two options were considered for modeling liquid phase tortuosity in the Models. The Millington-Quirk model is commonly used to estimate tortuosity in non-fractured porous media (Millington and Quirk, 1961) (see Jury and Horton, 2004, eq. 7.14, modified by division by water content for consistency with GoldSim.) The water phase tortuosity τ_w is calculated as

$$\tau_w = \frac{D_{eff}}{\theta_w D_{bulk}} = \frac{\theta_w^{7/3}}{n^2}. \quad (3)$$

An alternative estimate of tortuosity has been developed from an empirical relationship between D_{eff} and θ_w from measurements provided by Conca and Wright (1992). Effective diffusivities for over 300 samples were determined for NaCl and KCl solutions using their Unsaturated Flow Apparatus (UFA) to establish the water content and other physical conditions in the sample. The relationship between D_{eff} and θ_w for a range of soils and gravels is shown in Figure 1. The relationship is remarkably consistent over a wide range of materials, indicating that it is insensitive to the grain size of the porous medium.

The Conca and Wright (1992) model is expressed as a quadratic in log space:

$$\log_{10} D_{eff} = -4.1 + 2.7 \log_{10}(\theta_w) + 0.32 \log_{10}(\theta_w)^2. \quad (4)$$

Volumetric water content is expressed as a fraction and D_{eff} has implied units of cm^2/s . Using D_{bulk} of $2.03 \times 10^{-5} \text{ cm}^2/\text{s}$ for chloride (Domenico and Schwartz 1990, p. 369), water tortuosity can be estimated from equations (3) and (4) for all solutes:

$$\tau_w = \frac{D_{eff}}{\theta_w D_{bulk}} = \frac{10^{-4.1 + 2.7 \log_{10} \theta_w + 0.32 \log_{10} \theta_w^2}}{\theta_w 2.03 \times 10^{-5} \text{ cm}^2/\text{s}}. \quad (5)$$

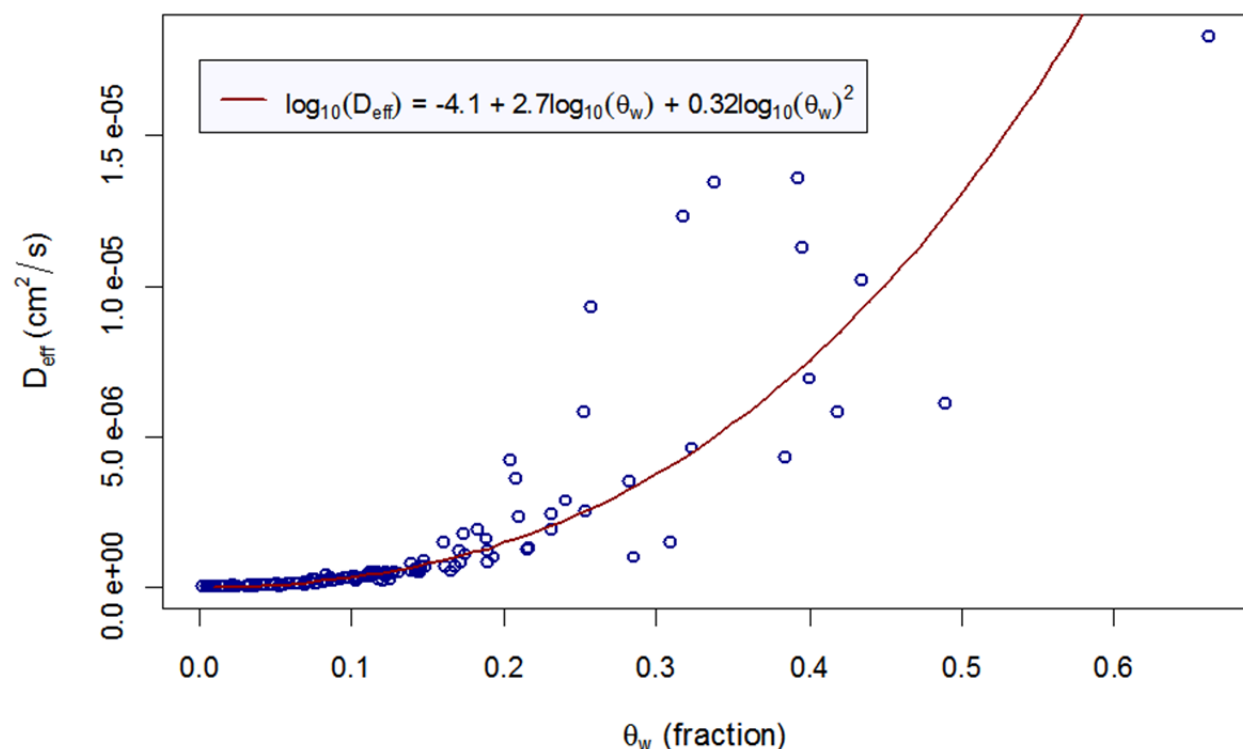


Figure 1. Estimated values of effective diffusivity D_{eff} for a range of volumetric water content for the Conca and Wright (1992) model. (After Conca and Wright, 1992).

The two tortuosity models are compared in Figure 2 using a representative effective porosity value of 0.37 for the Millington-Quirk model. Over the range of volumetric water contents from 0.10 to 0.20 the models differ by factors ranging from approximately 5 to 2.

Millington and Quirk (1961) concluded that, when considering porosity as the effective area of flow, the range on the porosity exponent in Equation (3) could be between 0.5 and 2 depending on the characteristics of the medium. There are physical constraints on the value of tortuosity. It can be seen from Equation (2) that the tortuosity of saturated porous media must always be less than $1/n$. When the tortuosity is equal to $1/n$ D_{eff} is equal to D_{bulk} and can never be larger. Although this is a physical upper limit to tortuosity, tortuosities measured in saturated porous media are always much smaller than $1/n$ and even smaller than $1/\theta_w$ for unsaturated media. Until the appropriate range can be determined, the exponents in the GoldSim model will be parameterized as normal distributions with a mean of 7/3 for the water content exponent and 2 for the porosity exponent and standard deviations of 0.001.

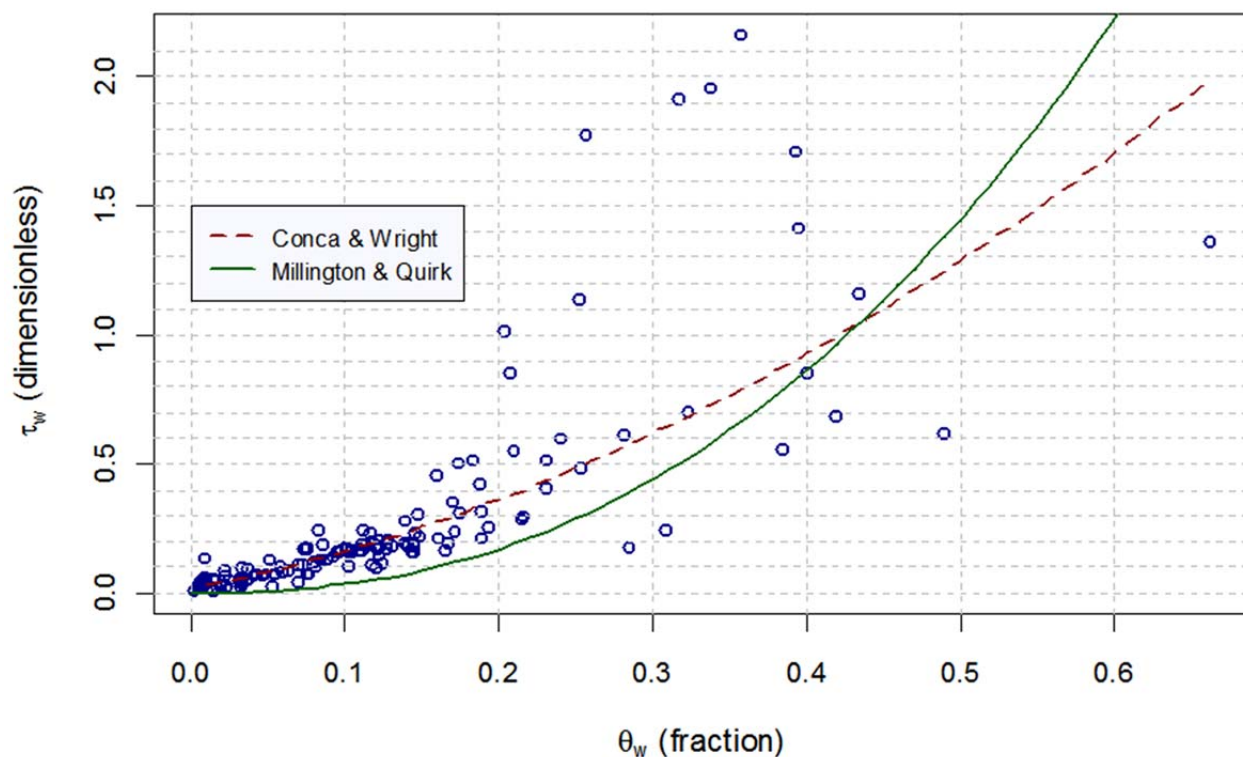


Figure 2. Water phase tortuosity function comparison between Millington-Quirk (Jin and Jury 1996) and Conca and Wright (1992).

4.0 Unsaturated Zone Air

The diffusion of volatile constituents in air is analogous to that of solutes in water, though the rates of diffusion are scaled by the free-air diffusivity (see the *Geochemical Modeling* white paper), and tortuosity is calculated differently, since air and water behave differently in pore spaces.

4.1 Diffusion in Air

Air-phase diffusion is included in the model, and this is the only process by which radionuclides are moved in the gas phase. The “built-in” diffusion calculations in GoldSim are used to estimate diffusion in the air phase. These gaseous diffusive fluxes are modified to handle unsaturated porous media (described in Section 4.2.2), but also include a calibration to counteract numerical dispersion for radon (discussed below in Section 4.3.3).

4.1.1 Atmospheric Boundary Condition

Diffusion in the air phase is modeled throughout the cover system, waste, and unsaturated subsurface hydrogeologic units bounded at the bottom by the saturated zone, and at the top by

the atmosphere. The bottom boundary condition is one of no diffusion, since there is no air in the saturated zone to diffuse into, by definition. The boundary condition at the top is effectively a zero-concentration sink, since the volume of air in the atmosphere flowing over the cover is sufficiently large that concentrations are kept much lower than in the pore air of the topsoil, cover, and wastes below. In order to model this, the air directly above the cover is represented by an Atmosphere Cell Pathway element in GoldSim. The volume of air is defined by a thickness times the area of the modeled column, and this air volume is flushed out by the wind. The diffusive flux from the uppermost cover cell in the column to the Atmosphere cell is defined by the diffusive area, as discussed above, and the diffusive length. Since the atmosphere is not a porous medium, a diffusive length unrelated to its thickness is adopted. Since the wind will maintain low concentrations in the atmosphere, amounting to a zero-concentration boundary condition, the choice of the parameters defining the Atmosphere is not expected to have much influence on the diffusive flux from the cover system. In order to verify this assumption, however, small uncertainties have been selected for these values, as shown in Table 1, in order to evaluate the model's sensitivity to them.

4.1.2 Air-Phase Tortuosity Models

A number of tortuosity models have been proposed for air phase diffusion in porous media. Using the form for tortuosity shown in (2) above, models reviewed by Jin and Jury (1996) include the Penman model (Penman, 1940) and two models attributed to Millington and Quirk.

In the Penman model, air phase tortuosity τ_a is a constant:

$$\tau_a = 0.66. \quad (6)$$

In the more commonly used Millington-Quirk model (MQ1), which is analogous to equation (3), tortuosity is expressed as

$$\tau_a = \frac{\theta_a^{7/3}}{n^2}. \quad (7)$$

And, in an alternative Millington-Quirk model (MQ2) evaluated by Jin and Jury (1996), tortuosity is expressed as

$$\tau_a = \frac{\theta_a}{n^{2/3}}. \quad (8)$$

Note that as θ_a approaches n (e.g. as the porous medium becomes drier), τ_a approaches $n^{1/3}$ for both formulations (7) and (8).

A three-porosity model (TPM) for gas phase tortuosity developed more recently by Moldrup et al. (2004) has been shown to provide more accurate estimates of gas phase tortuosity than the models above and was used in the WCS Site Model.

Gas-phase tortuosity for the TPM is given by Moldrup, et al. (2004) equation (12) as

$$\frac{D_{eff}}{D_{bulk}} = n^2 \left(\frac{\theta_a}{n} \right)^\chi \quad (9)$$

where the exponent χ is given in Moldrup, et al. (2004) equation (14):

$$\chi = \frac{\log_{10} \left(\frac{2 \theta_{a100}^3 + 0.04 \theta_{a100}}{n^2} \right)}{\log_{10} \left(\frac{\theta_{a100}}{n} \right)} \quad (10)$$

where

θ_{a100} is the air-filled porosity at -100 cm H₂O of matric potential.

4.1.3 GoldSim Implementation

In the notation used in GoldSim modeling, D_{eff}/D_{bulk} is the air-phase tortuosity τ_a times the air content θ_a . Therefore, the definition of the air- phase tortuosity used in GoldSim modeling is $\tau_a = (D_{eff}/D_{bulk})/\theta_a$, or

$$\tau_a = \frac{n^2}{\theta_a} \left(\frac{\theta_a}{n} \right)^{\left[\frac{\log_{10} \left(\frac{2 \theta_{a100}^3 + 0.04 \theta_{a100}}{n^2} \right)}{\log_{10} \left(\frac{\theta_{a100}}{n} \right)} \right]} \quad (11)$$

Tortuosity is implemented in the GoldSim model as a multiplier to the diffusive length, which is defined for each Cell Pathway element using the common method of setting it equal to 1/2 the cell length that is parallel to flow. In this case, that is the vertical dimension.

4.1.4 Estimation of θ_{a100}

An estimate of θ_{a100} for a material can be made by calculating the volumetric water content of the material at a matric potential of -100 cm using the van Genuchten soil-hydraulic model (van Genuchten, 1980 equations (2) and (3)) and the van Genuchten properties measured or estimated for that material. The volumetric water content is subtracted from the effective porosity giving θ_{a100} .

The van Genuchten model for water content as a function of matric potential is given by:

$$\theta(h) = \begin{cases} \theta_r + \frac{\theta_s - \theta_r}{[1 + |\alpha h|^n]^m} & h < 0 \\ \theta_s & h \geq 0 \end{cases} \quad (12)$$

where

θ_r	is the residual water content [-],
θ_s	is the saturated water content [-],
α	is a parameter [m^{-1}],
n	is a parameter [-],
m	is a parameter equal to $1-1/n$ with $n > 1$, and
h	is the matric potential [m].

4.2 Transport of Radon

A performance metric of the WCS Site Model is the ground surface flux of ^{222}Rn , and it is also a potential contributor to dose, so special attention is given its transport. Using a basic representation of fate and transport, radon emanation is accounted for, as is Henry's Law partitioning into water (see the *Geochemical Modeling* white paper), and the gas is allowed to diffuse in pore air using GoldSim's internal diffusion processes, as corrected for unsaturated media. Radon emanation is discussed below.

4.2.1 Radon Emanation (Escape/Production Ratio)

The fraction of ^{222}Rn produced by decay of radium-226 (^{226}Ra) that is released from the solid matrix is known as the escape-to-production (E/P) ratio, as well as the emanation coefficient, the emanation factor, or emanating power (Nielson and Sandquist, 2011). When ^{226}Ra decays, a small fraction of the decay energy, 0.1 MeV, is carried by the recoiling ^{222}Rn atom. This is sufficient energy for the recoiling atom to travel about 45 nm in a mineral matrix, 0.1 μm in water, and about 63 μm in air. Recoiling atoms with just sufficient energy to stop in the air or water filled pore space will be released from the matrix and become available for transport. If there is too little energy available, the atom will remain trapped in the solid matrix. If there is too much energy, the atom will cross the pore space and be embedded in the solid matrix of a nearby grain. The E/P ratio describes that fraction of ^{222}Rn that stops in the air or water-filled pore space and is free to diffuse. The E/P ratio can physically vary from a minimum of 0 to a maximum of 1.

Predicting the E/P ratio for a material is difficult as numerous factors have been identified that affect it: The E/P ratio is inversely related to grain size. The closer decaying atoms are to the surface of a grain, the more likely they will be released to the pore space. The adsorption or coprecipitation of ^{226}Ra on surficial coatings increases emanation, as will cracks, fissures, or pitting of grains. In contrast, the E/P ratio is directly related to pore size. As the pore size increases, it is more likely that recoiling atoms will stop in the pore space and emanation increases. The presence of water in the pore space increases emanation, because the reduced particle range in water increases the likelihood that the recoiling atom will stop in the pore space. Predicting the E/P ratio of a material is particularly difficult because it requires detailed knowledge of the microscopic physical structure of the material, microscopic distribution of ^{226}Ra in the material, and water content and distribution within a porous medium.

The E/P ratios for different types of common geologic materials have been reported. From geometrical considerations, the maximum emanation expected from a thick slab source is 0.5 and

from a thin film, 1.0. The maximum E/P ratio of natural solid materials will lie somewhere between these two extremes. The maximum value reported for common materials is approximately 0.7 to 0.8. Reported E/P ratios for soils and rocks range from 0.02 to 0.7 (UNSCEAR 2000; NCRP 1988). The emanation factor of a single material may vary over a substantial portion of this range depending on the water content. Rock and uncrushed ores usually have lower emanation factors ranging from 0.02 to 0.26 (Nazaroff 1992). Concrete emanation factors may range from 0 to 0.3 (Rogers et al. 1994; Cozmuta et al. 2003).

Nielson and Sandquist (2011, Table 1, p. 11) discuss radon modeling at length, and have assembled information about E/P ratios in uranium ores (in Table 1 of that document), which are reasonable analogs for uranium oxides that could be disposed at WCS. A placeholder normal distribution is chosen to represent the E/P ratio, with a mean of 0.2, with a standard deviation of 0.01 and truncated at 0 and 1.

For model regions outside the waste form, the E/P ratio is assumed to be 1. Since parents of radon may migrate within the model domain due to a number of contaminant transport processes, and may appear in various locations due to radioactive decay, ^{222}Rn may be produced outside the waste itself. For example, ^{226}Ra (or its parents) may have diffused up into the column, where it would be present in pore water and adsorbed to the surfaces of the porous media. Since this is not part of a mineral or other solid matrix, it is assumed that any radon produced through decay would likewise be immediately available for transport in pore air and water.

5.0 Saturated Zone Water

Transport in the porous medium water phase includes both advection and diffusion processes. Advective processes conceptually include infiltration of precipitation from the surface of the engineered cover, vertical downward flow through the unsaturated zone (including cover, waste, and the unsaturated zone above the 225-ft sandstone), flow through cover and waste layers, flow into the saturated 225-ft sandstone, and lateral flow in the 225-ft zone to a groundwater production well. As a result of the most recent INTERA modeling, however, the advection of water, including recharge to the saturated zone, is nonexistent under current climate conditions.

Diffusion is another principal contaminant transport process that is accounted for in the model. In the cover and waste layers, diffusion is modeled in both water and air phases, and is driven by concentration gradients within each phase as described above. If water is flowing quickly, advection and dispersion dominate diffusion, but if water flows slowly, or in the present case not at all, diffusion can play a significant role.

A legacy scenario presuming the use of the 225-ft sandstone as a drinking water source is included in the model. This calculation includes an estimate of well yield based on the Theim equation. Here the Theim equation is applied to the 225-ft saturated zone in order to estimate the rate at which water may be expected to be withdrawn from the well.

The presumed saturated zone (currently represented by the 225-ft sandstone member of the Dockum Group) underlies the entire site, and so has parameters and calculations that are global to all disposal units. Distributions were developed for two of the parameters used in the Theim equation: the saturated hydraulic conductivity, K_{sat} , and the borehole radius.

Twenty-one site-specific estimates of K_{sat} made in the 225-ft sandstone were used to determine a log-normal distribution with a geometric mean of 8.87×10^{-9} cm/s and a geometric standard deviation of 1.33. One outlier was removed prior to estimation, as the Coefficient of Variation was much more reasonable with the extremely high value removed. For estimation, the data was bootstrapped 1000 times and the resulting sampling distribution of the mean was inspected.

A distribution for the borehole radius was determined by first developing a distribution for well casing diameter for stock and domestic wells from the entries for stock and domestic wells in Andrews County, TX in the Texas Water Development Board Well Database. A Beta distribution was fit with a minimum of 1.5 in, a maximum of 12.5 in, a mean of 7.0 in, and a standard deviation of 2.1 in.

For the model, a casing diameter is chosen at random from the distribution and converted to a borehole diameter using a modified version of the relationship described in Roscoe Moss Company (2012) to account for the larger size of the borehole with respect to the casing. This conversion is equivalent to an 11.6 percent increase of the original casing diameter.

Since drill bits are manufactured in certain sizes, borehole sizes are calculated by applying the 11.6 percent correction described above to the calculation of the borehole diameter for the range of Andrews County well casings and rounding up to the nearest inch. Additional adjustments included a minimum diameter of 6 in and a minimum diameter increase of 2 in. The results in Table 2 of borehole diameters for the range of casing diameters reported for Andrews County used in the legacy scenario to represent flow to the well.

Table 2. Table of corresponding casing and borehole diameters.

Casing Diameter (in)	Borehole Diameter (in)
2	6
3	6
4	6
5	8
6	9
7	10
8	11
9	12
10	13
11	14
12	15

6.0 Material Properties

Porosity distributions for the materials in the modeled LLW column were provided in an email from Abhishek Singh (INTERA) to John Tauxe (Neptune and Company) dated 3 Oct 2012, subject: Dockum Porosities. These values, as well as dry bulk densities, are documented in the *Parameters Document*, formally entitled “*Parameters for the Model of the Waste Control Specialists Site, Andrews County, Texas WCS Site Model v0.205 (NAC-0005_R3)*.”

7.0 References

- Clennell, M.B. 1997. Tortuosity: a guide through the maze. in *Developments in Petrophysics*, Lovell, M.A. and P.K. Harvey (eds). Geological Society Special Publication No. 122, pp. 299-344.
- Conca, J.L., and J.V. Wright. 1992. Flow and Diffusion of Unsaturated Gravel, Soils and Whole Rock, *Applied Hydrogeology*, International Association of Hydrogeologists, Vol. 1, 1992, pp. 5-24.
- Cozmata, I., E. R. van der Graaf, and R. J. de Meijer, 2003. Moisture Dependence of Radon Transport in Concrete: Measurements and Modeling. *Health Physics* 85(4): 438 – 456.
- Domenico, P.A. and F.W. Schwartz. 1990. *Physical and Chemical Hydrogeology*. John Wiley & Sons, New York, NY.
- Freeze, R.A and J.A. Cherry. 1979. *Groundwater*. Prentice-Hall, Inc., Englewood Cliffs, NJ.
- GTG (GoldSim Technology Group). 2011. *User's Guide: GoldSim Contaminant Transport Module*, GoldSim Technology Group, Issaquah, WA, December 2010
- Hillel, D. 1980. *Fundamentals of Soil Physics*. Academic Press Inc. San Francisco, CA.
- Jin, Y., and W.A. Jury. 1996. Characterizing the Dependence of Gas Diffusion Coefficient on Soil Properties, *Soil Science Society of America Journal*, Vol. 60, pp. 66-71.
- Jury, W.A. and R. Horton. 2004. *Soil Physics*. 6th ed. John Wiley and Sons Inc. New Jersey.
- Koorevaar, P., G. Menelik, and C. Dirksen. 1983. *Elements of Soil Physics*. Elsevier. New York, NY.
- Marsily, G. de. 1986. *Quantitative Hydrogeology*. Academic Press Inc. San Diego, CA.
- Millington, R.J., and J.P. Quirk. 1961. "Permeability of porous solids." *Trans. Faraday Society* (57) pp. 1200-1207.
- Moldrup, P., T.Oleson, S. Yoshikawa, T. Komatsu, and D.E. Rolston. 2004. Three-porosity model for predicting the gas diffusion coefficient in undisturbed soil. *Soil Sci. Soc. Am. J.* 68:750-759. Madison, WI, USA.
- Nazaroff, W. W., 1992. Radon Transport from Soil to Air. *Rev. of Geophysics* 30(2): 137 – 162.
- NCRP (National Council on Radiation Protection and Measurements). 1988. *Measurements of Radon and Radon Daughters in Air*. NCRP Report No. 97, NCRP Bethesda, Maryland, November 1988.
- NRC (U.S. Nuclear Regulatory Commission). 1989. *Calculation of Radon Flux Attenuation by Earthen Uranium Mill Tailings Covers*, Regulatory Guide 3.64, Nuclear Regulatory Commission, June 1989.
- Nielson, K.K., and G.M. Sandquist. 2011. *Radon Emanation from Disposal of Depleted Uranium at Clive, Utah*. Report for EnergySolutions by Applied Science Professionals, LLC. February 2011.

- Nimmo, J.R., Deason, J.A., Izbicki, J.A., and Martin, P., 2002, Evaluation of unsaturated-zone water fluxes in heterogeneous alluvium at a Mojave Basin site: *Water Resources Research*, v. 38, no. 10, p.33-1 - 33-13.
- Penman, H.L. 1940. "Gas and vapor movements in the soil. I. The diffusion of vapors through porous solids." *Journal of Agricultural Science* (30) pp. 437-462.
- Rogers, V.C., K. K. Nielson, M. A. Lehto, and R. B. Holt. 1994. Radon Generation and Transport Through Concrete Foundations. EPA/600/SR-94/175, U. S. Environmental Protection Agency, Research Triangle Park, North Carolina, November 1994.
- Roscoe Moss Company. 2012. Borehole Diameter: How Large is Large Enough? Technical Memorandum 005-4, http://www.roscoemoss.com/pdfs/TechMemo005-4_Borehole_Diameter.pdf. Accessed 10/22/2012.
- Šimůnek, J., M. Šejna, H. Saito, M. Sakai, and M. Th. van Genuchten. 2009. The HYDRUS-1-D Software Package for Simulating the One-Dimensional Movement of Water, Heat, and Multiple Solutes in Variably-Saturated Media. Department of Environmental Sciences, University of California Riverside. Riverside, CA.
- UNSCEAR (United Nations Scientific Committee on the Effects of Atomic Radiation). 2000. UNSCEAR Report to the General Assembly – Sources and Effects of Ionizing Radiation.
- van Genuchten, M. Th. 1980. A closed form equation for predicting the hydraulic conductivity of unsaturated soils. *Soil Sci. Soc. Am. J.* 44:892-898. Madison, WI, USA.
- WCS. 2007. Application for License to Authorize Near-Surface Land Disposal of Low-Level Radioactive Waste, Revision 12c, Waste Control Specialists, Dallas, TX, 1 May 2007.
- WCS. 2011. Updated Performance Assessment for the Low-Level Waste Facility, Waste Control Specialists, Dallas, TX, 17 October 2011.