REDUCTION IN UNCERTAINTY IN THE GEOLOGIC SETTING PERFORMANCE MEASURE, 10 CFR 60.113(a)(2): COMPUTER CODE SELECTIONS, CONCEPTUAL MODELS, AND DATABASES

a **⁰**

Prepared for

Nuclear Regulatory Commission Contract NRC-02-88-005

Prepared by

George Rice Ronald Green Jeffrey Pohle

Center for Nuclear Waste Regulatory Analyses San Antonio, Texas

September 1993

CONTENTS

 \sim \sim $\label{eq:2} \frac{1}{\sqrt{2}}\sum_{i=1}^n\frac{1}{\sqrt{2}}\sum_{i=1}^n\frac{1}{\sqrt{2}}\sum_{i=1}^n\frac{1}{\sqrt{2}}\sum_{i=1}^n\frac{1}{\sqrt{2}}\sum_{i=1}^n\frac{1}{\sqrt{2}}\sum_{i=1}^n\frac{1}{\sqrt{2}}\sum_{i=1}^n\frac{1}{\sqrt{2}}\sum_{i=1}^n\frac{1}{\sqrt{2}}\sum_{i=1}^n\frac{1}{\sqrt{2}}\sum_{i=1}^n\frac{1}{\sqrt{2}}\sum_{i=1}^n\frac{1$

 $\ddot{}$

0

FIGURES

 $\label{eq:2} \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}\right)^{2} \left(\frac{1}{\sqrt{2}}\right)^{2}$

 \mathcal{L}^{\pm}

0

TABLES

Table Page 3-1 3-2 3-3 3-4 *3-5* 3-6 3-7 3-8 3-9 Summary of property values for basalt geologic setting 3-3 ... Property value ranges and document sources for basalt geologic setting 3-5 Summary of property values for granite geologic setting $\ldots \ldots \ldots \ldots \ldots$ 3-7 Property value ranges and document sources for granite geologic setting 3-8 Summary of property values for salt geologic setting 3-10 Property value ranges and document sources for salt geologic setting 3-11 Summary of property values for conceptual model (a) $-$ tuff geologic setting 3-13 Summary of property values for conceptual model (b) $-$ tuff geologic setting 3-16 Property value ranges and document sources for tuff geologic setting 3-20 ...

ACKNOWLEDGMENTS

This report was prepared to document work performed by the Center for Nuclear Waste Regulatory Analyses (CNWRA) for the U.S. Nuclear Regulatory Commission (NRC) under Contract No. NRC-02-88-005. The activities reported here were performed on behalf of the NRC Office of Nuclear Material Safety and Safeguards (NMSS), Division of High-Level Waste Management (DHLWM). The report is an independent product of the CNWRA and does not necessarily reflect the views or regulatory position of the NRC. The authors wish to thank Dr. Gordon Wittmeyer for his technical review and Dr. Budhi Sagar for his editorial review of this document.

1 INTRODUCTION

Systematic Regulatory Analyses (SRA) has identified several Key Technical Uncertainties (KTU) in the performance measure for the Geologic Setting (GS) described in 10 CFR 60.113(a)(2). The NRC is investigating various avenues, such as rule making and/or staff guidance, for reducing these uncertainties. Numerical exploration of any modification to the Ground Water Travel Time (GWTT) rule in 10 CFR 60.113(a)(2) is an essential component of such investigations. The objective of the numerical analyses will be to test the ability of the proposed modifications to evaluate the goodness of the site to isolate waste. Specifically, the modifications under consideration are: (i) calculation of GWTT under post-closure anticipated conditions, rather than pre-waste-emplacement conditions; (ii) starting from the mid-plane of the repository rather than the edge of the disturbed zone; and (iii) specification of some percentile for compliance rather than the fastest path.

This report summarizes the identification of computer codes selected for these computational analyses, and the compilation of the conceptual models and databases used to define the geologic scenarios for which the proposed performance measure will be assessed. In order to maintain the generic nature of the rule, the proposed measure will be applied to four different geologic settings, each with properties appropriate for individual generic sites. These are: (i) basalt; (ii) granite; (iii) salt; and (iv) tuff. These four geologic settings are thought to represent most probable sites of the proposed geologic high-level waste (HLW) repository. The first three geologic settings are identified as being hydraulically saturated and the fourth, tuff, is identified as being hydraulically unsaturated/saturated. High permeable fault zones will be included in the granite conceptual model to provide for an assessment of their effect on the GS performance measure.

2 COMPUTER CODE SELECTION

Computational analyses will be conducted to calculate the performance measure for the GS for both prewaste-emplacement and anticipated post-waste-emplacement conditions. Analyses conducted for pre-wasteemplacement conditions will provide a measure of the performance of each GS for existing conditions. Anticipated post-waste-emplacement conditions are defined to include only the thermal effect of waste emplacement and the mechanically disruptive effect of repository construction upon the flow of groundwater. Geochemical and geochemical-mechanical effects will not be addressed during the evaluation of the performance measure for the GS. These two classes of processes are source term dependent and their effects will be assessed as part of the performance measure of the overall system (10 CFR 60.112).

The flow of groundwater from the repository to the accessible environment under both saturated and unsaturated conditions and in response to the thermal effects of waste emplacement will be calculated as part of this exercise. Therefore, the computer codes selected to perform the analyses will need to track water through isothermal and nonisothermal, saturated and unsaturated media. No single computer code will be used to perform all aspects of the analyses for all geologic settings. In general, one computer code will be used to determine the groundwater flow field for a particular geologic setting and a second code will be used to track groundwater particles through the determined flow field.

Three computer codes have been selected to calculate the groundwater flow regime for the geologic settings under isothermal/nonisothermal saturated conditions. These three codes are PORFLOW (Runchal and Sagar, 1993), V-TOUGH (Pruess, 1987; Nitao, 1990) and SWIFT III (Ward et al., 1993). The selection of the code that will be used for a particular setting will be made at the time the analyses are initiated. It may be determined that the use of all three codes in this analysis is not necessary since evaluation of the different codes is not an objective of this task. Code selection will be made based upon the merits of the code and the needs of the model application to the particular geologic setting.

V-TOUGH has been selected as the computer code to be used to model groundwater flow through the unsaturated portion of the tuff geologic setting. V-TOUGH or one of the two other computer codes mentioned above for modeling saturated flow will be used to model the saturated portion of the tuff geologic setting scenario.

The travel time of individual water particles will be tracked for the groundwater flow regimes calculated for each of the geologic settings using a particle-tracking computer code. Two codes have been identified for the analysis, SLIM (Tompson et al., 1987) and PARTICLE (Gureghian et al., 1987). Selection of the particle-tracking computer code for each application will be made when the conceptual models are incorporated into numerical models. An alternative computer code will be identified and used if initial computer code choices for calculating either groundwater flow or particle movement prove untenable or unfeasible.

3 CONCEPTUAL MODELS AND DATABASES

* **0**

Conceptual models for the four geologic settings have been identified. Numerical models for each of the four settings will be constructed based on the conceptual models. Although the conceptual models are intended to be generic site representations of the four geologic settings, three of the conceptual models, with the exception of the granite geologic setting, are based upon actual geographical locations, the B-WIPP site at Hanford, WA for the basalt scenario, the WIPP site at Carlsbad, NM for the salt site, and Yucca Mountain, NV for the tuff geologic setting. This similarity is attributed to the following two reasons. First, the conceptual models for the basalt, salt, and tuff geologic settings are from locations that at some time have been under consideration as potential sites for the HLW repository. This implies that these sites possess characteristics that are, in general, consistent with the construction of a HLW repository and that any sites representative of these geologic settings would possess similar characteristics. Second, because of the availability of earlier studies related to the emplacement of a HLW repository at these three sites, a significant amount of information on these sites is available for the modeling analyses. The conceptual model for the fourth geologic setting, granite, is not based upon an actual geographic location. It is modeled after a massive batholith with no particular identifying features.

Included with each conceptual model are two tables containing property values for the geologic setting. One table contains the reasonable range of values for each variable of interest. References to the source documents for these property values are identified by an assigned number in this table. The other table contains a summary of a reasonable value for each of the variables for use in assigning properties in the numerical models. These selected values are intended to be initial values only and may be re-evaluated and changed during the modeling exercise.

Following are descriptions of the conceptual models and the associated databases for the four geologic settings. An alternative conceptual model for the tuff scenario is also included. This alternative conceptual model is expanded at depth to include a carbonate aquifer. Selection of the appropriate model will be made during execution of the analysis.

3.1 BASALT GEOLOGIC SETTING

The repository is excavated in the middle of a 40-m-thick, dense interior zone of a basalt flow (Figure 3-1). The basalt conceptual model is based upon Davis et al. (1989), Bonano et al. (1989), and Isherwood (1981). Included in the conceptual model figure are several points (A,B,...) where initial values for hydraulic head and temperature are specified. The interior zone is 1,000 M below land surface and is bounded above and below by 10-m-thick basalt interflow zones. Both interflow zones are bounded by other basalt flows. These flows extend for hundreds of meters above the upper interflow and hundreds of meters below the lower interflow. The structure of the dense zone consists of vertical hexagonal columns that formed as the basalt cooled. The columns are approximately 1 m in diameter, and the fractures that bound the columns provide the most permeable pathways within the interior zone. The interflow zones contain vesicles, small diameter columns, and horizontal fractures such that the interflow zones are several orders of magnitude more permeable than the dense interior.

All three zones are under hydraulically confined conditions. Groundwater flow in the interflow zones is horizontal. These zones are recharged at their outcrops and discharge to streams. The recharge

 $=$ Groundwater Flow Direction

Figure 3-1. Basalt conceptual model

and discharge areas are many kilometers from the area of interest. Groundwater flow in the dense interior zone is vertically upward. It is recharged by the lower interflow zone and discharges to the upper interflow zone. A summary of the property values for the basalt geologic setting is presented in Table 3-1. The ranges for these values and their document sources are presented in Table 3-2.

Table 3-1. Summary of property values for basalt geologic setting

 \sim $\label{eq:2} \frac{1}{2} \left(\frac{1}{2} \right)^{2} \left(\frac{1}{2} \right)^{2} \left(\frac{1}{2} \right)^{2}$

Table 3-1. Summary of property values for basalt geologic setting (Cont'd)

Table 3-2. Property value ranges and document sources for basalt geologic setting. Document sources are: (1) Isherwood (1981), (2) Mercer et al. (1982), (4) Bonano et al. (1989), and (5) Davis et al., (1989).

 \mathbf{r}

 $\ddot{}$

 $\frac{1}{2} \sum_{i=1}^{n} \frac{1}{2} \sum_{j=1}^{n} \frac{1}{2} \sum_{j=1}^{n$

3.2 GRANITE GEOLOGIC SETTING

0

The repository is excavated in a granitic batholith 1,000 m below land surface (Figure 3-2). The information base upon which the granite conceptual model was formulated was taken from a compendium of different geographical provinces most of which are located in the western United States (Isherwood, 1981). Included in the conceptual model figure are several points (A,B,...) where initial values for hydraulic heat and temperature are specified. The granitic rock extends from land surface to several kilometers below the repository. It contains several intersecting fracture systems and groundwater flows almost exclusively along these fractures. A limited number of fault zones will be incorporated into the model to provide for an assessment of their effect on the performance measure. The fracture zone permeability is assumed to be several orders of magnitude greater than the matrix permeability. The fault zone is assigned a porosity of 10 percent. Groundwater flow through the matrix in the vicinity of the repository is horizontal from the repository to its accessible boundary and the flow system may be confined or unconfined. Groundwater flow in the fracture zone is assumed to be in the direction of the fault zones. The recharge and discharge areas are many kilometers from the area of interest. A summary of the property values for the granite geologic setting are presented in Table 3-3. The ranges for these values and their document sources are presented in Table 3-4.

- = Groundwater Flow Direction

Figure 3-2. Granite conceptual model

Table 3-3. Summary of **property** values **for** granite geologic setting

 $\bar{\mathcal{A}}$

 \mathcal{L}_{max}

Table 3-3. Summary of property values for granite geologic setting (Cont'd)

Table 3-4. Property value ranges and document sources for granite geologic setting. Document sources are: (1) Isherwood (1981), and (2) Mercer et al. (1982).

Property	Range	Document Source	Representative Value	Document Source
Hydraulic conductivity - matrix	$8.6 E-13 - 3.8 E-9$ m/s	$1 - V2$, p 304	$1.0 E-11 m/s$	$1 - V2$, p 315
Hydraulic conductivity $-$ fractured	$2.0 E-11 - 4.6 E-5$ m/s	$1 - V2$, p 304	$1.0 E-9 m/s$	$1 - V2$, p 315
Porosity	$0.07 - 3\%$	$1 - V2$, p 304	1%	$1 - V2$, p 304
Density	$2520 - 2810$ kg/m ³	2, p 127	2670 kg/m^3	2, p 127
Dispersivity - longitudinal (fractured schist-gneiss)			134.1 m	$1 - VI$, p 212
Thermal conductivity	$1.51 - 4.48$ $W/m-C$	$1 - V2$, p 258	3.25 W/m-C	$2 - p$ 118
Specific heat	804 - 1009 J/kg-C	$2 - p$ 125, $1 - V2$, p 266	990 J/kg-C	$1 - V2$, p 264
Thermal diffusivity			1.47 E-6 m^2/s	$1 - V2$, p 296

3.3 SALT GEOLOGIC SETTING

The repository is excavated in the middle of a bed of salt (Figure 3-3). The salt conceptual model is based upon Cranwell et al. (1990), Isherwood (1981), and Mercer et al. (1982). Included in the conceptual model figure are several points (A,B,...) where initial values for hydraulic head and temperature are specified. It is approximately 1,000 m below land surface. The salt bed is composed of halite and bounded above and below by beds of dolomite. The units above the upper dolomite bed and below the lower dolomite bed are composed of interbedded salt and dolomite. These units extend to the surface and more than 1,000 m below the lower dolomite bed.

All three beds are confined. Groundwater flow in the dolomite is horizontal. The dolomites are recharged at their outcrops and discharge to streams. The recharge and discharge areas are many kilometers from the area of interest. Groundwater flow in the salt bed is vertically upward. It is recharged by the lower dolomite and discharges to the upper dolomite. A summary of the property values for the salt geologic setting is presented in Table 3-5. The ranges for these values and their document sources are presented in Table 3-6.

 $=$ Groundwater Flow Direction

Figure 3-3. Salt conceptual model

Table 3-5. Summary of property values for salt geologic setting

0

 \sim

 $\ddot{}$

 $\ddot{}$

Table 3-5. Summary of property values for salt geologic setting (Cont'd)

* **S**

Table 3-6. Property value ranges and document sources for salt geologic setting. Document sources are: (1) Isherwood (1981), (2) Mercer et al. (1982), (3) Weast (1981), (4) Bonano et al. (1989), (7) Cranwell et al. (1990), and (8) Freeze and Cherry (1979).

Table 3-6. Property value ranges and document sources for salt geologic setting (Cont'd)

3.4 TUFF GEOLOGIC SETTING

The conceptual model for the tuff geologic setting is described in Section 3.4.1. The tuff (a) model extends from ground surface to 50 m below the water table for a total depth of 600 m. An alternative model, tuff (b), has been included. This conceptual model extends to a total depth of 1600 m, of which the lower-most 50-m-thick layer consists of limestone. The selection of the appropriate model for the tuff geologic setting will be made during execution of the analyses. The tuff conceptual models are based upon Guzowski et al. (1983); Tien et al. (1985); NRC (1993); and DOE (1988).

A summary of the property values for the tuff geologic setting conceptual model (a) and conceptual model (b) are presented in Tables 3-7 and 3-8, respectively. The ranges for these values and their document sources are presented in Table 3-9.

3.4.1 Conceptual Model (a)

The repository is excavated in unsaturated tuff (Figure 3-4). Included in the conceptual model figure are several points (A,B,...) where initial values for hydraulic heat and temperature are specified. The repository is 300 m below land surface and 250 m above the water table. The water table aquifer is also composed of tuff. The tuff extends to over 1,000 m below the water table. All the tuff in the vicinity of the repository is fractured and water may flow through both the fractures and the matrix.

. **0**

Recharge to the unsaturated zone is appointed as 1 mm/yr and flow in this zone is essentially vertical. Flow in the water table aquifer is horizontal. This aquifer receives most of its recharge at its outcrop and discharges to springs. The recharge and discharge areas are many kilometers from the area of interest.

Table 3-7. Summary of property values for conceptual model (a) - tuff geologic setting

Table 3-7. Summary of property values for conceptual model (a) — tuff geologic setting (Cont'd)

* **0**

Table 3-7. Summary of property values for conceptual model (a) - tuff geologic setting (Cont'd)

 $\ddot{}$

 \bar{z}

 $\hat{\mathbf{r}}$

Table 3-7. Summary of property values for conceptual model (a) - tuff geologic setting (Cont'd)

0 ⁰

Table 3-8. Summary of property values for conceptual model (b) — tuff geologic setting

Table 3-8. Summary of property values for conceptual model (b) - tuff geologic setting (Cont'd)

 $\bar{\beta}$

Table 3-8. Summary of property values for conceptual model (b) - tuff geologic setting (Cont'd)

 $\ddot{}$

Table 3-8. Summary of property values for conceptual model (b) - tuff geologic setting (Cont'd)

 $\ddot{}$

 \mathcal{L}

Table 3-9. Property value ranges and document sources for tuff geologic setting. Document sources are: (1) Isherwood (1981), (2) Mercer et al. (1982), (3) Weast (1981), (8) Freeze and Cherry (1979), (9) NRC (1993), (10) Guzowski et al. (1983), and (11) Tien et al. (1985).

* **S**

Table 3-9. Property value ranges and document sources for tuff geologic setting (Cont'd)

 \sim \star

 $\ddot{}$

 \sim \sim

= Groundwater Flow Direction

Figure 3-4. Tuff conceptual model (a)

3.4.2 Conceptual model (b)

The repository is excavated in unsaturated tuff (Figure 3-5). Included in the conceptual model figure are several points (A,B,...) where initial values for hydraulic heat and temperature are specified. The repository is 300 m below land surface and 250 m above the water table. The water table aquifer is also composed of tuff. All the tuff in the vicinity of the repository is fractured and water may flow through both the fractures and the matrix. The tuff extends 1,000 m below the water table and is measured by a confined limestone aquifer.

Recharge to the unsaturated zone averages 1 mm/yr and flow in this zone is vertical. Flow in the water table aquifer is vertical. This aquifer receives its recharge from the unsaturated zone and discharges to the underlying limestone aquifer. The limestone aquifer receives most of its recharge from its outcrop and discharges to springs. The recharge and discharge areas are many kilometers from the area of interest.

= Groundwater Flow Direction

Figure 3-5. **Tuff conceptual model (b)**

4 REFERENCES

- Bonano, E.J., P.A. Davis, L.A. Shipers, K.F. Brinster, W.E. Beyeler, C.D. Updergraff, E.R. Shepherd, L.M. Tilton, and K.K. Wahi. 1989. *Demonstration of a Performance Assessment Methodology for Level Radioactive Waste Disposal in BasaltFormations.* NUREG/CR-4759, SAND86-2325. Washington, DC: U.S. Nuclear Regulatory Commission.
- Cranwell, R.M., R.W. Guzowski, J.E. Campbell, and N.R. Ortiz. 1990. *Risk Methodology for Geologic Disposal of Radioactive Waste, Scenario Selection Procedure.* NUREG/CR-1167, SAND80-1429. Washington, DC: U.S. Nuclear Regulatory Commission.
- Davis, P., W. Beyeler, M. Logston, N. Coleman, and K. Brinsten. 1989. *Numerical Modeling of Ground Water Flow Systems in the Vicinity of the Reference Repository Location, Hanford Site, Washington.* NUREG/CR-5089, SAND88-0141. Washington, DC: U.S. Nuclear Regulatory Commission.
- Freeze, R.A., and J.A. Cherry. 1979. *Groundwater.* Edgewood Cliffs, NJ: Prentice Hall, Inc.
- Gureghian, A.B., A. Andrews, S.B. Steidl, and A. Brandstetter. 1987. *Solutions to ROCOIN Level I Problems (Cases 1, 2, 4, 7) using STOKES and PARTICLE.* BMI/OCRD28. Columbus, OH: Battelle Memorial Institute: Office of Crystalline Repository Development.
- Guzowski, R.V., Nimick, F.B., M.D. Siegel, and N.C. Finley. 1983. *Repository Site Data for Tuff: Yucca Mountain, Nevada.* NUREG/CR-2937, SAND82-2105. Washington, DC: U.S. Nuclear Regulatory Commission.
- Isherwood, D. 1981. *Geoscience Data Base for Modeling a Nuclear Waste Repository.* NUREG/CR-0912, Volumes 1 and 2. Washington, DC: U.S. Nuclear Regulatory Commission.
- Mercer, J.W., S.D. Thomas, and B. Ross. 1982. *Parameters and Variables Appearing in Repository Siting Models.* NUREG/CR-3066. Washington, DC: U.S. Nuclear Regulatory Commission.
- Nitao, J.J. 1990. *VTOUGH: An Enhanced Version of the TOUGH Code for the Thermal and Hydrologic Simulation of Large Scale Problems in Nuclear Waste Isolation.* UCID-21954. Livermore, CA: Lawrence Livermore National Laboratory.
- Pruess, K. 1987. *TOUGH User's Guide.* NUREG/CR-4645. Washington, DC: U.S. Nuclear Regulatory Commission.
- Runchal, A.K., and B. Sagar. 1993. *PORFLOW: A Multiflow Multiphase Model for Simulating Flow, Heat Transfer, and Mass Transport in Fractured Porous Media.* NUREG/CR-5991, CNWRA 92-003. Washington, DC: U.S. Nuclear Regulatory Commission.
- Tien, P.-L., M.D. Siegel, C.D. Updegraff, K.K. Wahi, and R.V. Guzowski. 1985. *Repository Site Data Report for Unsaturated Tuff, Yucca Mountain, Nevada.* NUREG/CR-4110, SAND84-2668. Washington, DC: U.S. Nuclear Regulatory Commission.
- Tompson, A.F.B., E.G. Vomvoris, and L.W. Gelhar. 1987. *Numerical Simulation of Solute Transport in Randomly Heterogeneous Porous Media.- Motivation, Model Development, and Application.* UCID-21281. Livermore, CA: Lawrence Livermore National Laboratory.
- U.S. Department of Energy. 1988. *Site Characterization Plan.* Yucca Mountain Site, Nevada Research and Development Area, Nevada, Volume II, Part A, Chapter 3. DOE/RW0199.
- U.S. Nuclear Regulatory Commission. 1993. *Phase 2 Demonstration of the NRC's Capability to Conduct a Performance Assessment for a Level Waste Repository.* NUREG-1464. Washington, DC: U.S. Nuclear Regulatory Commission. In preparation.
- Ward, D.S., A.L. Harrover and A.H. Vincent. 1993. *Data Input Guide for SWIFT/486, Release 2.53.* Sterling, VA: GEOTRANS.
- Weast, R.C., ed. 1981. *CRC Handbook of Chemistry and Physics, 60th Edition.* Boca Raton, FL: CRC Press, Inc.