~~XXXX~~ RMIS View/Print Document Cover Sheet ~~XXXX~~

This document was retrieved from the Documentation and Records Management (DRM) ISEARCH System. It is intended for Information only and may not be the most recent or updated version. Contact a Document Service Center (see Hanford Info for locations) if you need additional retrieval information.

Accession #: D195062845

Document #: SD-WM-RPT-189

Title/Desc:

DEVELOPMENT OF A UNIT CELL MODEL FOR INTERIM
PERFORMANCE ASSESSMENT OF VITRIFIED LLW DISPOSAL

Pages: 81

NOV 21 1995
5.34, 73

ENGINEERING DATA TRANSMITTAL

Page 1 of 1
1. EDT 603221

2. To: (Receiving Organization) Distribution		3. From: (Originating Organization) Administrative Systems Resources (62400)		4. Related EDT No.: NA	
5. Proj./Prog./Dept./Div.: LLW		6. Cog. Engr.: N. W. Kline		7. Purchase Order No.: NA	
8. Originator Remarks:				9. Equip./Component No.: NA	
				10. System/Bldg./Facility: NA	
11. Receiver Remarks:				12. Major Assm. Dwg. No.: NA	
				13. Permit/Permit Application No.: NA	
				14. Required Response Date: 10/26/95	

15. DATA TRANSMITTED					(F)	(G)	(H)	(I)
(A) Item No.	(B) Document/Drawing No.	(C) Sheet No.	(D) Rev. No.	(E) Title or Description of Data Transmitted	Approval Designator	Reason for Transmittal	Originator Disposition	Receiver Disposition
1	WHC-SD-WM-RPT-189		0	Development of a Unit Cell Model for Interim Performance Assessment of Vitrified Low Level Waste Disposal	NA	1	1	1

16. KEY			
Approval Designator (F)	Reason for Transmittal (G)		Disposition (H) & (I)
E, S, Q, D or N/A (see WHC-CM-3-5, Sec. 12.7)	1. Approval 2. Release 3. Information	4. Review 5. Post-Review 6. Dist. (Receipt Acknow. Required)	1. Approved 2. Approved w/comment 3. Disapproved w/comment 4. Reviewed no/comment 5. Reviewed w/comment 6. Receipt acknowledged

(G)	(H)	17. SIGNATURE/DISTRIBUTION (See Approval Designator for required signatures)				(G)	(H)
Reason	Disp.	(J) Name	(K) Signature	(L) Date	(M) MSIN	Reason	Disp.
1	1	Cog. Eng. N. W. Kline		10/26/95	NO-36		
1	1	Cog. Mgr. F. K. Mangan		11/2/95	NO-22		
		QA					
		Safety					
		Env.					
1	1	R. Khaleel		11/1/95	NO-36		
1	1	F. M. Mann		11/2/95	NO-36		

18. N. W. Kline Signature of EDT Originator Date 10/26/95		19. F. M. Mann Authorized Representative Date 11/2/95 for Receiving Organization		20. F. K. Mangan Cognizant Manager Date 11/2/95		21. DOE APPROVAL (if required) Ctrl. No. ☐ Approved ☐ Approved w/comments ☐ Disapproved w/comments	
--	--	--	--	--	--	---	--

RELEASE AUTHORIZATION

Document Number: WHC-SD-WM-RPT-189, Rev. 0

Document Title: Development of a Unit Cell Model for Interim
Performance Assessment of Vitrified Low Level Waste
Disposal

Release Date: 11/13/95

**This document was reviewed following the
procedures described in WHC-CM-3-4 and is:**

APPROVED FOR PUBLIC RELEASE

WHC Information Release Administration Specialist:

V. L. Birkland
V. L. Birkland

11/13/95

TRADEMARK DISCLAIMER. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof or its contractors or subcontractors.

To obtain copies of this report, contact:

Westinghouse Hanford Company - Document Control Services
P.O. Box 1970, Mailstop H6-08, Richland, WA 99352
Telephone: (509) 372-2420; Fax: (509) 376-4989

SUPPORTING DOCUMENT1. Total Pages **77**

2. Title

Development of a Unit Cell Model for Interim
Performance Assessment of Vitrified Low Level
Waste Disposal

3. Number

WHC-SD-WM-RPT-189

4. Rev No.

0

5. Key Words

Low Level Waste Disposal
Performance Assessment
Vadose Zone
Flow and Transport Modeling

6. Author

Name: **N.W. Kline**Signature **10/26/95**Organization/Charge Code **8H620/D4DC1**

7. Abstract

A unit cell model has been developed and used in analysis of some design options for a vitrified low level waste disposal facility. The unit cell modeling approach is likely to be useful in interim performance assessment for the facility. The present unit cell model will probably need to be refitted in terms of some model parameters for the latter purpose.

Two present disposal facility concepts differ substantially in the length of a capillary barrier proposed to limit effective recharge through the top of the facility. Results of analytical study, experimental observation, and numerical simulation reviewed and summarized herein suggest that design of a capillary barrier which can reduce a recharge rate of 0.1 cm/yr by one or even two orders of magnitude seems feasible for both concepts. Capillary barrier effectiveness is subsequently treated as a parameter for the recharge boundary condition in the unit cell model.

The unit cell model for predicting performance of a LLW glass disposal facility is based on simulated performance of a single one of the proposed thousands of waste packages to be emplaced in the disposal facility. A benchmark comparison of the unit cell model against a full facility model shows that the unit cell model can provide comparable predictive accuracy in less than one percent of the computer time.

In the present application to disposal system design options, results from the unit cell model suggest that capillary barrier performance is one of the more important model parameters. Other parameters to which the model shows some sensitivity of disposal system performance include inter-canister spacing, rate of moisture withdrawal due to glass corrosion, contaminant inventory, and the well intercept factor. It is also important that variations of waste form hydraulic parameters suggest that transport through the waste form is dominated by diffusion.

8. RELEASE STAMP

DEVELOPMENT OF A UNIT CELL MODEL FOR INTERIM PERFORMANCE ASSESSMENT OF VITRIFIED LOW LEVEL WASTE DISPOSAL

September 1995

Prepared By:

N.W. Kline
Fellow Software Engineer
BCS Richland, Inc.

Date: 10/26/95

Reviewed By:

F.M. Mann
Fellow Scientist
Westinghouse Hanford Company

Date: 11/2/95

TABLE OF CONTENTS

1.0	INTRODUCTION	1
2.0	CAPILLARY BARRIER MODEL	2
2.1	BACKGROUND	2
2.2	NUMERICAL MODEL	6
3.0	UNIT CELL MODEL	11
3.1	UNIT CELL APPROACH	11
3.2	BASE CASE FLOW AND TRANSPORT	11
3.3	RESULTS AND DISCUSSION	13
3.3.1	Concept 1: 10 cm Inter-Canister Spacing	13
3.3.2	Concept 2: 35 cm Inter-Canister Spacing	13
3.3.3	Capillary Barrier: $a=0.1$	14
3.3.4	Capillary Barrier: $a=0.01$	14
3.3.5	Intact Concrete Floor: Step-Change to Gravel at 1000 Years	14
3.3.6	Concrete Floor: Minimum Conductivity Cutoff = 10^{-20}	14
3.3.7	Lo-QC Sand Filler	15
3.3.8	Sandy Gravel Waste Form	15
3.3.9	Side Influx: 100% Return of Diverted Moisture ($a=0.1$)	16
3.3.10	Side Influx: 50% Return of Diverted Moisture ($a=0.1$)	16
3.3.11	Capillary Barrier: $a=0.1$ with Minimum $k_r = 10^{-20}$	16
3.3.12	Moisture Withdrawal: $a=0.1$ and Minimum $k_r = 10^{-20}$	16
3.3.13	Sandy/Gravel Waste Form: Minimum $k_r = 10^{-20}$	17
3.3.14	Effect of Initial Conditions: Minimum $k_r = 10^{-20}$	17
3.3.15	Tc-99 Transport Properties in the Waste Form	17
3.3.16	Well Intercept Factor	18
3.3.17	Inventory	18
3.3.18	Summary of Dose Results	19
4.0	SUMMARY AND CONCLUSIONS	21
5.0	REFERENCES	24

TABLES

1.	Slope-Length Combinations for Barrier Simulations	7
2.	Hydraulic Properties of Materials	8
3.	Summary of Simulated Capillary Barrier Efficiencies	9
4.	Comparison of Peak Doses	20

FIGURES

1.	Schematic Diagram of Capillary Barrier Model	27
2.	Steady-State Effective Saturation for Hi-QC Capillary Barrier with 5% Slope under 0.1 cm/yr Recharge	28
3.	Steady-State Effective Saturation for Hi-QC Capillary Barrier with 20% Slope under 0.1 cm/yr Recharge	29
4.	Characteristic Curves for Sand and Gravel Barrier Materials	30
5.	Schematic Drawing of Unit Cell Model	31
6.	Steady-State Saturation Distribution with Streamlines	32
7.	Comparison of Peak Doses from Concept 1 and Concept 2	33
8.	Reduction of Drinking Doses due to Capillary Barrier Effectiveness	34
9.	Bulk Rates of Change of Volumetric Moisture Content in the Waste Form	35
10.	Characteristic Curves for Gravel and Five Sandy Gravel Sediment Samples	36
11.	Decrease in Dose with Decrease in Return of Moisture Diverted by a Capillary Barrier	37
12.	Effect of Moisture Withdrawal due to Corrosion	38
13.	Principal Contributors to Base Case Drinking Water Dose	39

APPENDIX

APPENDIX A	A-1
----------------------	-----

ACKNOWLEDGEMENTS

The assistance of Scott Finfrock, Westinghouse Hanford Company, in helping run the numerical simulations of capillary barrier performance and in reviewing an early draft of this report is gratefully acknowledged. The author wishes to thank Mel Piepho, Daniel B. Stephens & Associates, Inc., for providing PORFLOW input files for the full facility models and for providing the GRTPA dose code input files. Appreciation is also expressed for review comments, stimulating discussions, and useful references provided by Allen Lu and Raz Khaleel, Westinghouse Hanford Company.

TRADEMARK ACKNOWLEDGEMENTS

PORFLO-3 and PORFLOW are trademarks of Analytic and Computational Research, Inc., Los Angeles, California.

IBM and RISC System/6000 are registered trademarks of International Business Machines Corporation, Armonk, New York.

Silicon Graphics is a trademark of Silicon Graphics, Inc., Mountain View, California.

1.0 INTRODUCTION

In accordance with the Tri-Party Agreement (Ecology et al., 1994), the U.S. Department of Energy (DOE) and Westinghouse Hanford Company (WHC) are proceeding with engineering work in support of the disposal of radioactive waste that is stored on the Hanford Site in southcentral Washington State. Much of the waste is in the form of liquids and precipitated sludges that are presently stored in single-shell and double-shell underground tanks. Following retrieval and pretreatment of the waste, the low level waste (LLW) fraction will be vitrified and disposed in an onsite near-surface facility.

Approval of an approved site-specific Performance Assessment (PA) of the disposal facility is required by DOE Order 5820.2A (DOE, 1988). The purpose of the PA is to provide reasonable assurance that public health and the environment will be protected in accordance with applicable local, state and federal regulations. An Interim Performance Assessment (IPA), although not required, is being developed to show prior to any facility construction that there will be a high likelihood of approvability of the Final PA. The IPA is also intended to provide technical guidance to the facility design.

The purpose here is to describe the development of a "unit-cell" model for use in assessing facility performance, and to present some initial results produced in support of a revision to a report on disposal system design options (Rawlins et. al 1994). The unit-cell modeling approach is also intended to be of use in support of the IPA, although the present unit-cell model described herein will likely need to be refitted in terms of stratigraphy, material properties and boundary conditions for that particular application.

The term "unit-cell" is used to relate that waste isolation performance of the facility is evaluated based on simulated performance of a single one of the proposed 6804 waste canisters to be emplaced in the facility (Eiholzer 1995). The primary performance indicator evaluated by the model is radiation dose from all radionuclide species in drinking water drawn from the aquifer at a well 100 meters downgradient from the facility. Other performance indicators evaluated by the model presently include radiation dose from using irrigation water, radiation dose due to radon production, and radiation dose due to intrusion. The model also provides estimates of arrival concentrations and fractional release rates at the water table of the uppermost aquifer system along with travel times to the water table for water and contaminants. Initial results given here are presented in terms of the drinking water dose indicator. A benchmark against a full facility model for a base case provides some initial assurance that the unit-cell simulation approach provides sufficient accuracy. It is important to note that the model results reported herein are intended primarily to demonstrate how the model works, not how well the disposal system performs, for the disposal system is presently only in the preconceptual design stage of development (Eiholzer 1995).

2.0 CAPILLARY BARRIER MODEL

2.1 BACKGROUND

Physical dimensions and elevations of the proposed disposal facility along with proposed spatial arrangements of waste canisters in the facility under two current concepts have been established for use in developing the IPA (Eiholzer 1995). For both concepts, a Hanford-type surface barrier (Myers and Duranceau, 1994) having top surface even with existing grade will be used to limit recharge due to precipitation. The expected soil moisture recharge rate beneath the Hanford-type barrier due to net infiltration of precipitation through the barrier ranges from about 0.05 cm/yr up to about 0.3 cm/yr (Rockhold et al, 1995). For the present work, the recharge rate is assumed to be 0.1 cm/yr (1 mm of water per year) for consistency with the design options study (Rawlins et al, 1994).

Below the Hanford-type barrier there will be a secondary capillary barrier to further reduce the influx of moisture through the top surface of the disposal facility. The capillary barrier is composed of fine soil overlying coarser soil. At equilibrium, capillary pressure in the finer soil will adjust to a value at which the infiltration rate equals the hydraulic conductivity (Ross 1990). The underlying coarser material will equilibrate to a similar potential. As long as the moisture content of the two materials is sufficiently small, the hydraulic conductivity of the coarser material will be negligible or at least small compared to the hydraulic conductivity of the finer material. Infiltrating moisture will therefore diffuse preferentially in the finer soil above the contact with the coarser soil. The capillary barrier is so named because the controlling physical mechanism is the capillary pressure developed in the finer soil.

The contact between the fine soil and the coarse underlying soil of the capillary barrier will be sloped down from a central point to promote drainage of the barrier away from the facility (such as shown in Figure 1). One of the fundamental differences between the two competing facility concepts is in capillary barrier length (Eiholzer 1995). Under equilibrium conditions, the effective length of one side of a capillary barrier has been shown by Ross (1990) to be bounded by

$$L < \frac{K_s \tan A}{q\alpha}, \quad (1)$$

where K_s is the saturated hydraulic conductivity of the fine soil,

A is the angle of inclination of the soil layer contact from the horizontal,

q is the net infiltration rate of precipitation, and

α is the fitting parameter from the exponential characteristic for unsaturated hydraulic conductivity of the fine soil; i.e.,

the unsaturated hydraulic conductivity of the fine soil is taken to follow approximately the exponential relationship

$$K = K_s e^{\alpha \psi} \quad (2)$$

with ψ representing the capillary pressure. Noting that $\tan A$ is simply the slope of the capillary barrier (i.e. $\tan A = H/L$ where H is the total rise in the barrier along the length L as in Figure 1), then equation (1) for the effective length becomes

$$L < [HK_s / q \alpha]^{0.5} \quad (3)$$

Equation (3) is a convenient form from which to estimate necessary rise for a barrier of some fixed length; i.e., $H > L^2 q \alpha / K_s$.

The exponential conductivity characteristic parameter α can be determined by using the fact that the relative hydraulic conductivity is

$$k_r = K/K_s = e^{\alpha \psi} \quad (4)$$

in which case

$$\alpha = (\ln k_r) / \psi \quad (5)$$

As an example, assume that the fine soil for the capillary barrier is the same as Sample 241-AP-1 from the Upper Hanford formation at the AP Tank Farm in the 200 East Area. That particular sample is 98% sand and 2% silt by weight, after particles of size greater than 2 mm were sieved out. Analysis of the 241-AP-1 soil sample appears in appendices of a report by Smoot et al. (1989). Under the assumed equilibrium conditions in the capillary barrier, the unsaturated conductivity of the fine soil is $K = q = 0.1 \text{ cm/yr} = 3 \times 10^{-9} \text{ cm/sec}$. The saturated hydraulic conductivity is $K_s = 0.0026 \text{ cm/s}$, and hence at the assumed recharge rate the relative conductivity is $k_r = 1.2 \times 10^{-6}$. Also, under the equilibrium assumption, $K=q$, the volumetric moisture content is near the residual value at about $\theta = 0.04$ and the capillary pressure head is approximately $\psi = -100 \text{ cm}$ as determined graphically from characteristic curves (e.g. in Smoot et al, 1989). Hence equation (5) gives $\alpha = 0.14 \text{ cm}^{-1}$. From Eiholzer (1995) the slope of the capillary barrier under Concept 1 is 3%; i.e., $\tan A = 0.03$. Therefore, the effective length of the capillary barrier under the proposed Concept 1 with the fine soil assumed to be represented by the 241-AP-1 soil sample is not more than about 1800 meters on one side from equation (1). This example estimate is comparable to one given by Ross (1990), taking into account the difference in assumed recharge rate, even though the two fine soils considered here and there are dissimilar in terms of their respective hydraulic parameters. For clarity, it should also be noted that $L=1800 \text{ m}$ in this example is an estimate of maximum effective length for one side of a barrier that is peaked in the center. Total effective barrier length for the two-sided barrier is $2L$, equal to about 3.6 km (about 2 mi) for the present example.

For the preceding discussion and example it has been clearly assumed that the infiltration rate q is constant and that fluid pressures above and below the soil layer contact are at equilibrium. But even with the Hanford-type barrier

in place over the capillary barrier, field scale infiltration into the capillary barrier is likely to be episodic. Further analyses by Steenhuis et al. (1991) and Ross (1991) agree that nonequilibrium conditions produced by periodic wetting and drying can improve the capillary barrier performance in terms of the effective length L .

Stormont (1995) further improves upon the Ross (1990) estimate of capillary barrier performance by including the effect of constant anisotropy of the hydraulic conductivity. For the present purpose, the anisotropy of the hydraulic conductivity can be taken to be the ratio of the lateral component of conductivity (in the fine soil parallel to the contact) to the transverse component of conductivity (in the fine soil perpendicular to the contact). Generally the anisotropy of hydraulic conductivity in an unsaturated medium is dependent upon moisture content, even in a homogeneous soil (McCord et al., 1991), and typically increases with decreasing moisture content (Yeh et al., 1985a & 1985b; Stephens and Heermann, 1988; McCord et al, 1991; Kline and Khaleel 1995). Thus low moisture content should further enhance the function of the capillary barrier by producing an anisotropic hydraulic conductivity field in the barrier. Conductivity variations in thinly layered fine soils can also induce anisotropy; Yeh et al (1985b) show that this is because the unsaturated anisotropy depends in part upon the variance of K_s within the layered system. Yeh et al (1985c) recommend a barrier system composed of layers of differently textured materials; this is largely the principle of the Hanford-type barrier which not only diverts moisture but also retains it for later removal by evapotranspiration (Myers and Duranceau, 1995).

Theoretical performance of capillary barriers as addressed by Ross (1990), Morel-Seytoux (1994), Stormont (1995), and others is typically focused on effective length as exemplified above by equations (1) and (3). It is also of interest to have some estimate of required thickness of the fine soil layer. Ross (1990) proceeded by calculating downdip flux of water, finding the region along the contact where downdip flux increases sharply and limiting the effective length to the point downdip where flux across the barrier becomes equal to the recharge rate. For that approach the soil layer thickness does not enter the calculations. For the anisotropic case, Stormont (1995) assumed that the thickness of the fine layer, b , satisfies

$$b > N(\alpha \cos A)^{-1} \quad (6)$$

where N is a small integer (i.e., "a few"). Ross (1990) introduced the above thickness criterion as the approximate thickness at which inequality (1) should hold with equality. Inequality (6) reduces to $b > N/\alpha$ for small angle A . For the preceding example with the fine soil having properties of the sieved 241-AP-1 soil sample, the required thickness is only about $b > 20$ cm for $N=3$ and still less than a meter thickness even for $N=10$. But for the Ross (1990) example, the required thickness according to criterion (6) is on the order of a few meters, even though the two soil types considered provide a similar effective length L at $q = 0.1$ cm/yr.

Morel-Seytoux (1994) showed that the effective capillary barrier length for an "excellent" barrier is equivalent to the Ross (1990) length estimate in equation (1). An "excellent" barrier is one in which flux across the contact

along the entire effective length is "much less" than the recharge rate. Morel-Seytoux (1994) points out that the improvement to the Ross (1990) analysis by Steenhuis et al (1991) provides the reason why the length estimate in equation (1) is applicable to an "excellent" capillary barrier. In the analysis by Morel-Seytoux (1994), the thickness of the fine soil layer in the excellent barrier is assumed to be "relatively small", i.e., "18 to 24 inches." This thickness assumption is consistent with the thickness of less than a meter for the example with 241-AP-1 fine soil.

Field-scale observations of performance of a capillary barrier in East Wenatchee, Washington for about a two-year period showed favorable comparison to a traditional resistive barrier (Khire et al., 1994). The resistive barrier is composed of a 60 cm thick layer of compacted silty clay overlain by a 15 cm thick layer of silty clay. The resistive barrier functions simply by presenting a layer of reduced permeability in the path of infiltrating precipitation - an obstacle which sheds moisture, similarly to the shedding effect of an underground single-shell tank (Kline and Khaleel, 1995). The capillary barrier in the experiment is composed of a 75 cm thick sand (coarse) layer overlain by a 15 cm thick silt (fine) layer, and functions as described earlier in this section. Each test barrier covers an area 30 m by 30 m with no slope. Both barriers are subject to in situ conditions and natural precipitation which is typically in the range of 20 to 30 cm/yr. Khire et al. (1994) report that the moisture content of both barriers increases dramatically in Winter due to seasonal precipitation and then decreases through the Spring, Summer and Fall as a result of evapotranspiration (similarly to the Hanford-type barrier). They also report that during the Winter wetting period the silt (fine) layer of the capillary barrier becomes "nearly saturated", but that the water content of the underlying sand (coarse) layer increases only "moderately". These results suggest that the capillary barrier effect is realized with a relatively thin (15 cm thick) fine layer and no slope to promote drainage. In comparison of the two barriers, Khire et al. (1994) report that the resistive barrier of length $L=30$ m allowed twice the rate of seepage through the barrier as did the capillary barrier of length $L=30$ m. The experimental capillary barrier allowed about 1% of precipitation across the barrier whereas the resistive barrier allowed about 2% of precipitation across the barrier.

Some mixing of the fine and coarse soil particles at the contact between the layers of a capillary barrier is inevitable, but the difference in hydraulic conductivity between the fine and coarse materials should still serve to divert some infiltrating moisture laterally. This makes the point that the thickness of the layers in the capillary barrier might be important not only to initial performance but also to the effective lifetime of the barrier. For instance, in the facility specifications for the IPA (Eiholzer 1995), aside from the natural porosity of materials used in facility construction there is a specification that each of the 6804 2m x 2m x 8m waste canisters will have a 5% void space at one end (the "top" end). The total void volume due thereto is over 10,000 cubic meters. The average eventual subsidence over the area of the entire facility under assumption of Concept 1 dimensions is about 30 cm (about 1 foot), due entirely to proposed intentional voids in the waste canisters. So although analysis of an excellent barrier and short-term observation of an experimental barrier seem to indicate that a relatively thinly layered and low-sloped capillary barrier can be an effective device in

limiting infiltration, the fine and coarse layers of the capillary barrier might need to be thicker than suggested earlier in this section to promote longevity of the barrier in the face of potential canister collapse, subsidence and soil mixing.

2.2 NUMERICAL MODEL

Two-dimensional and three-dimensional numerical simulations of capillary barrier performance in diverting flow around a hypothetical concrete vault have recently been reported by Nichols and Meyer (1995). Their results suggest that performance of a capillary barrier of fixed length $L=28$ m is "highly sensitive" to properties of barrier materials, but not to slope of the contact between the fine and coarse layers. In light of the theory, examples and experiment described in Section 2.1, it is expected that performance of a capillary barrier of length $L=28$ m might not be sensitive to variations in slope from 4% to 20% as used in the simulations. For instance, using fine soil represented by the 241-AP-1 soil sample for a barrier of length $L=28$ m with a recharge rate of $q=0.1$ cm/yr, the required rise for an excellent barrier as obtained from application of equation (2) is only about $H=1$ cm ($\tan A=4.5 \times 10^{-4}$). However, Nichols and Meyer (1995) were investigating barrier performance under a high recharge condition of $q=32$ cm/yr (roughly twice the local average annual precipitation), and their simulations included effects of varying hydraulic properties of both the fine and coarse materials as well as comparison of accuracy between two-dimensional and three-dimensional finite element based simulations. The purpose in this section is to describe related finite difference based simulations including some of the same property and slope variations as Nichols and Meyer (1995), and also extend the work to lower recharge rates and longer barrier lengths for consistency with modelling to be performed in support of the upcoming IPA.

The present capillary barrier simulations are based on a two-dimensional modeling approach. This is consistent with the conclusions by Nichols and Meyer (1995) that two-dimensional modeling of a capillary barrier system can be more conservative than three-dimensional modeling in terms of flux admitted through the barrier, and that the two-dimensional modeling approach should be sufficient for a performance assessment. A schematic diagram of the spatial arrangement for the present simulations is shown in Figure 1. The entire domain is represented by a homogeneous fine soil except for a wedge of coarser soil as shown in the figure. For each simulation case, the total rise of the wedge is $H=10$ m and the slope of the inclined contact between the fine and coarse soils is varied by changing the length, L . The slopes used for the present simulation cases and the corresponding lengths are shown below in Table 1. Hydraulic properties of fine and coarse materials used for the

various simulation cases are shown in Table 2. Note that the values of the parameter α given in Table 2 are for the van Genuchten (1980) characteristic rather than the exponential conductivity characteristic shown in equation 2.

Table 1. Slope-Length Combinations for Barrier Simulations.

Slope H/L	2.5%	5%	10%	20%
Length L	400 m	200 m	100 m	50 m
Angle A	1.43°	2.86°	5.71°	11.31°
# Nodes	8	4	2	1

The capillary barrier simulations reported here were run using Version 1.2 of the finite difference based PORFLO-3 code (Runchal et al., 1992) as implemented (Kline, 1994) on the WHC Scientific and Engineering Computational Center (SECC). For all cases the node spacing vertically through the wedge of coarse material is $\Delta z = 1$ m. The base grid has 101 equally spaced nodes laterally ($\Delta x = 5$ m). The grid aspect ratio ($\Delta x / \Delta z$) is constant at a value of 5 over most of the domain; it decreases to a value of 1 along the bottom, and increases up to a value of 10 along the top two layers of nodes. For most of the simulation cases the total height of the domain was 30 m as shown in Figure 1 and the total length was 500 m. For some of the cases with steep slope (short wedge length) the total length of the domain (in the x-direction) was shortened correspondingly for computational efficiency. For some of the cases with high recharge the total height of the domain was extended below $z = -30$ m for improved numerical convergence. The higher recharge cases exhibited good barrier effectiveness and therefore higher downdip flux which resulted in a steeper moisture gradient into the shadow under the wedge. This necessitated the vertical extension of the domain below the wedge to minimize errors along the fixed head boundary at the bottom of the domain (cf. Figure 1).

Table 2. Hydraulic Properties of Materials.

Soil	α cm ⁻¹	n	K _s cm/s	θ_s	θ_r	Source
241-AP-1	0.1008	2.9224	2.55x10 ⁻³	0.417	0.0322	a
Hi-QC Sand	0.0683	2.080	3x10 ⁻²	0.37	0.045	b
Mid-QC Sand	0.0440	1.523	3x10 ⁻²	0.35	0.098	b
Lo-QC Sand	0.0440	1.523	1x10 ⁻⁴	0.35	0.098	b
Hi-QC Gravel	3.5366	2.661	1.85	0.51	0.014	b
Mid-QC Gravel	0.4	2.922	1	0.34	0.02	b
Gravel ^(*)	3.5366	2.661	1.85	0.518	0.014	c
Backfill ^(**)	0.0683	2.080	3x10 ⁻²	0.371	0.045	c
241-AP-1g	0.1018	2.9473	1.2x10 ⁻³	0.26	0.021	a,c
Hanford Sand	0.1943	1.868	1.55x10 ⁻³	0.4203	0.0234	c
Hanford Gravel	0.0290	1.613	2.73x10 ⁻⁴	0.3584	0.0213	c
Ringold	0.0176	1.338	2.42x10 ⁻⁶	0.4982	0.0283	c
Concrete	7.61x10 ⁻⁶	1.393	3.75x10 ⁻¹⁰	0.2258	0	c

- a Smoot et al, 1989
b Nichols and Meyer, 1995
c Khaleel and Freeman, 1995

- * Gravel^c = Hi-QC Gravel^b
** Backfill^c = Hi-QC Sand^b

Simulations were run with values of recharge ranging from the 32 cm/yr value used by Nichols and Meyer (1995) down to 0.01 cm/yr. A simulation was executed for each of the four slope-length combinations from Table 1 at each recharge rate. In addition, some variation of hydraulic properties was included in simulations at the 0.1 cm/yr recharge rate. Each simulation was based on either Hi-QC sand surrounding Hi-QC gravel or Mid-QC sand around Mid-QC gravel. Barrier efficiency was calculated from the results of each simulation. Those results are summarized below in Table 3. The barrier efficiency is calculated in terms of the difference between the fluid volume entering the domain due to recharge above the barrier and fluid volume from flux across the contact between the fine and coarse soils; i.e.,

$$\text{Efficiency} = (1 - V_2/V_1) \times 100\% \quad (7)$$

where $V_1 = qL\Delta y$ is fluid volume due to recharge,
 $V_2 = \Delta x \Delta y \sum_{i=2,m} w_i$ is fluid volume crossing the barrier,

w_i is vertical flux through the contact at node x_i ,
 m is the number of nodes along the length L , and
 $\Delta y = 1 \text{ m}$ is the thickness of the 2D planar domain.

Table 3. Summary of Simulated Capillary Barrier Efficiencies.

Attributes	Slope=2.5%	Slope=5%	Slope=10%	Slope=20%
q=0.01, Hi-QC	99.9%	99.9%	99.9%	99.9%
q=0.1, Hi-QC	99.9%	99.9%	99.9%	99.9%
q=0.1, Mid-QC	99.9%	99.9%	99.9%	99.9%
q=1, Hi-QC	99.9%	99.9%	99.9%	99.9%
q=10, Hi-QC	99.9%	99.9%	99.9%	99.9%
q=32, Hi-QC	99.9%	99.9%	99.9%	99.9%

All of the simulations obtained near-perfect efficiency, i.e., near 100% of infiltration is shed off of the barrier in each simulated case. This is not unexpected in light of the length estimate given by equation 1 for an excellent barrier and the example given in Section 1.1. Moreover, the efficiency results shown in Table 3 replicate efficiencies of Hi-QC barriers at all slopes from the work reported by Nichols and Meyer (1995). The use of Mid-QC sand and gravel versus use of Hi-QC sand and gravel is unremarkable at the 0.1 cm/yr recharge rate. This contrasts with some sensitivity to material properties at the high recharge rate of 32 cm/yr in the Nichols and Meyer (1995) study. In general terms, as the recharge rate increases from a very low value, differences between conductivities of a pair of fine and coarse barrier materials become smaller. Eventually there is typically a recharge rate at which the conductivities are equal and the coarse layer is no longer a barrier. This is referred to as the crossover point for the pair of conductivity characteristics. Further increases in recharge rate will cause the coarse material to become more conductive than the fine material. For the particular case of no reportable sensitivity of barrier efficiency to materials at the recharge rate of 0.1 cm/yr contrasted with high sensitivity of barrier efficiency at the high recharge rate of 32 cm/yr, it suffices to note that the crossover point for the Hi-QC materials is about $2 \times 10^{-2} \text{ cm/s}$, the crossover point for the Mid-QC materials is slightly lower at about 10^{-2} cm/s , and the crossover point for the Lo-QC materials is about $2 \times 10^{-6} \text{ cm/s}$ - only slightly above the 32 cm/yr (10^{-6} cm/s) recharge rate. These crossover points are estimated from inspection of the conductivity characteristic curves shown as Figure 4 in the Nichols and Meyer (1995) paper and reproduced here as Figure 4. Note that in Figure 4 the sand characteristic curves are marked by an "S" and the gravel characteristics are unlabeled. The conductivity characteristics suggest that barrier efficiency should be good for the Hi-QC materials and almost as good for the Mid-QC materials over the range of recharge rates used here. The characteristics in

Figure 4 also suggest almost no barrier effectiveness for the Lo-QC materials at the 32 cm/yr recharge rate, but that efficiency should improve with decreasing recharge rate. This observation is consistent with simulation results reported here.

A fundamental difference between the simulations reported here and those reported by Nichols and Meyer (1995) is that their results were obtained by representing the sloping contact exactly in a finite element grid with nonrectangular elements while the simulations reported here employed a finite difference grid of rectangular elements to represent the contact as a sequence of 10 "stairsteps" over the barrier length. (The last row of Table 1 shows the number of nodes laterally per stairstep.) An important result is that exact (smooth) versus approximate (stairstep) representation of the contact is not important to the simulated efficiency for the present cases. The stairsteps can be apparent in contours of steady-state pressure heads or moisture contents such as shown in Figure 2. For the high slope, short length case shown in Figure 3, the stairsteps are not readily apparent. This is because there is one node per step (cf. Table 1), and the contouring software connects the dry gravel nodes creating an apparent diagonal contact. Both cases, Figures 2 and 3, show the accumulation of moisture along the contact and bending of streamlines across the contact. In the limit as the angle of inclination A goes to 90° , the contact should become a streamline. For the cases represented by Figures 2 and 3 the contact does not appear to be a streamline, but it should be noted that apparent lateral diversion of the streamlines at the contact in these figures is diminished due to relative compression of the horizontal axis.

3.0 UNIT CELL MODEL

3.1 UNIT CELL APPROACH

The unit cell model presented here is patterned after the performance model used in the Grout PA (Kincaid et al., 1995). The stratigraphy, material properties and boundary conditions are largely the same as used for the Grout PA model. The contaminant source term is the same as used by Rawlins et al (1994) in their study of LLW glass disposal system design options. The computer codes used to run the model, Version 2.394gr of PORFLOW and Version 3.0 of GRTPA, are from the same Grout PA Code System (GPACS) which has been tested by Piepho et al (1994). The innovation in the unit cell modeling approach is that the source term is represented spatially by a quadrant of a single waste canister instead of a full facility cross-section. Moreover, the upper boundary of the model is the top of the facility, a meter above the top of the waste canister (Eiholder 1995). The effects of the surface barrier and capillary barrier are included accordingly with results provided in the previous section. In effect the model is one-dimensional except for the filler between canisters as shown in Figure 5. The result of the unit cell approach is a model with number of nodes about two orders of magnitude less than in the predecessor models developed for the Grout PA (Kincaid et al., 1995) and LLW disposal design options study (Rawlins et al., 1994). In terms of computation, the model runs a 100,000 year simulation in a matter of minutes rather than the hours or days taken for the full-facility models. Hence the unit cell approach is well-suited for efficiently running the many simulation cases that are foreseen in the support of design analyses and development of the IPA. The particular version of the unit cell model presented here will likely need some refitting for application in the IPA.

3.2 BASE CASE FLOW AND TRANSPORT

The source term representation in the unit cell model is a vertical quadrant of one of the 2 m by 2 m by 8 m tall canisters described by Eiholder (1995). The "left" side of the model is a vertical axis of symmetry through a one-meter-thick slice of a single canister. The "right" side of the model is a vertical axis of symmetry through the filler between two canisters. The canister region shown in the model schematic diagram in Figure 5 is 1 m wide by 1 m thick by 8 m high. The only difference between Concept 1 and Concept 2 in the unit cell model is the thickness of the filler region between canisters. The inter-canister spacing is 10 cm for Concept 1 and 35 cm for Concept 2 (Eiholder 1995). Hence the model width (in the x-direction) is 1.05 m for Concept 1 and 1.175 m for Concept 2.

For the base case with both Concepts 1 and 2, the engineered structures (i.e., vault, canister and waste form) are assumed to be short-lived compared to the 100,000 year time span covered by the performance simulations. No credit is taken for waste isolation capability of the vault or canister. The waste form ("canister" region in Figure 5) is assumed to be fractured to the extent that it behaves hydraulically like gravel (Hi-QC gravel). The filler material between and overlying canisters in the vault serves at least initially to prevent collapse of the vault ceiling and subsidence of the capillary and

surface barriers. But the filler material should also serve to divert infiltrating moisture around the canisters - another capillary barrier. The base case hydraulic properties of the filler are taken to be backfill (Hi-QC sand). Spatially the remainder of the model is the vadose zone from the bottom of the vault down through the upper and lower Hanford formation sequences to the approximate elevation of the water table in the Ringold Formation. All of the base case material property assignments are the same as used for the central analysis case described by Rawlins et al (1994) [cf. Table 2].

The sides of the model are axes of symmetry; the left side represents symmetry about the center of a canister and the right side represents symmetry about the center of the filler between two canisters (cf. Figure 5). The top of the model corresponds to the elevation of the top of the vault walls. Contaminant concentration is assumed to be zero at that elevation. Influx of moisture through the top of the model (a-q) is assumed to be proportional to the assumed recharge rate through the bottom of the surface barrier ($q=0.1$ cm/yr). For the base case simulations, the constant of proportionality is $a=1$; i.e., no credit is taken for the effect of the capillary barrier in the base case. The water table is represented at the bottom of the model by zero pressure head and zero total head (at $z = 0$). Transport of contaminants through the vadose zone from the waste form to the water table and into the unconfined aquifer is assumed to be dominated by advection. Correspondingly, the transport boundary condition at the water table is zero diffusive flux. The simulated base case steady state flow field based on these conditions is shown in Figure 6. The initial conditions for the steady state run were derived from the unit gradient assumption (Khaleel and LeGore 1990).

Seventy percent of the volume of each canister is assumed to be glass cullet. The remainder of the canister volume is assumed to be fractured sulphur polymer cement. Release of contaminants in the waste form due to dissolution of the glassified waste by infiltrating moisture is assumed to be congruent in time with the reduction of small glass spheres of initial radius 0.25 cm at a constant rate of 10^{-5} cm/yr along the radius. This results in an effective release period of 25,000 years. Note that this release scenario determines a fractional release rate of contaminant mass within the source zone (canister region in Figure 5). All contaminant mass from the dissolution of the LLW glass is assumed to have become available for transport within the source region within 25,000 years; however, contaminant mass concentrations in water inside the source region and contaminant mass flux out of the source region are determined in part by the availability of contaminant and also by the availability of moisture as the host for diffusive and advective transport.

Base case inventories of contaminants as well as contaminant transport properties such as distribution coefficient (K_d) are taken initially to be the same as in the central analysis case of Rawlins et al (1994). This is for the purpose of benchmarking the present unit cell model against the more detailed models in terms of previously reported drinking water doses. Using the same well-intercept factor and GRTPA dose code input from the central analysis case with the present Concept 1 base case obtains a peak drinking water dose of 147 mrem/yr at about 8600 years due to drinking water derived from a well

100 meters downgradient from the glass waste disposal facility. This compares closely to the results of the central analysis case (cf. Figure 3 by Rawlins et al., 1994).

The essential difference between the previous central analysis case (Rawlins et al., 1994) and the present Concept 1 base case is the spatial representation of the source term. Whereas the source term was represented by a vault full of glass beads for the former and by one-quarter of a canister for the latter, they both provide similar results in terms of drinking water dose. However, the generic vault model required on the order of hours of cpu time to run with the GPACS on an IBM RISC System/6000 Model 580 while the canister model took about five cpu minutes to run with the same codes on the same computer.

Another more recent full facility model based on the Concept 1 dimensions of Eiholzer (1995) was developed independently (Piepho 1995) and has been run with the same base case parameters described here for comparative results. The new full facility model predicted a Concept 1 base case maximum dose of about 145 mrem/yr between about 8,000 and 9,000 years after time of disposal. This result also compares well with the unit cell model results for the Concept 1 base case and the central analysis case. The full facility Concept 1 base case simulation as run with the GPACS on an IBM RISC System/6000 Model 580 required about 12 hours cpu time, and took over two days elapsed time because of heavy demand. The same simulation running on a Silicon Graphics Indigo required about 15 hours cpu time and only slightly longer elapsed time.

3.3 RESULTS AND DISCUSSION

The results contained here were obtained from simulations run with the unit cell model using the GPACS on the WHC SECC. Each simulation case represents a variation of the Concept 1 base case described above in Section 3.2. Only one parameter is varied from one case to the next. Results of each case are summarized in terms of the drinking water dose for comparison of the effects of the various cases.

3.3.1 Concept 1: 10 cm Inter-Canister Spacing

The present Concept 1 base case as described above in Section 3.2 with 10 cm spacing between canisters gives a peak dose of about 147 mrem/yr at about 8600 years. This is obtained using the inventory and well-intercept factor from the central analysis case reported by Rawlins et al (1994).

3.3.2 Concept 2: 35 cm Inter-Canister Spacing

Concept 2 with 35 cm of filler between canisters gives a peak dose of about 112 mrem/yr at 9,000 years after time of disposal. Concept 1 and Concept 2 drinking water doses are compared in Figure 7. The peak dose from Concept 2 is decreased and slightly delayed compared to the peak dose from Concept 1 because of the extra volume of filler between canisters. The filler over the

canisters can act as a capillary barrier to divert infiltrating moisture away from the top of the waste form as shown by the streamlines in Figure 6. The extra volume of filler between canisters results in lower expected volumetric moisture content in the filler and hence higher tension and lower hydraulic conductivity.

A simple hand calculation based on two canisters and the intervening filler and assuming $q=0.1$ cm/yr at the top of the vault but with a 100% effective local capillary barrier over each canister due to the contrast between properties of the filler and the waste form suggests that the replacement of moisture in the filler between canisters is about three times faster with the 10 cm inter-canister spacing as compared to the 35 cm spacing.

Lower moisture content is expected to lower the release rate, and slower moisture movement is expected to delay the time of peak occurrence.

3.3.3 Capillary Barrier: $a=0.1$

Concept 1 with a capillary barrier which reduces the net recharge rate through the top of the vault to 0.01 cm/yr produces a peak dose of about 32 mrem/yr at 40,000 years, as shown in Figure 8.

3.3.4 Capillary Barrier: $a=0.01$

Reduction of recharge to 0.001 cm/yr through the top of the vault results in further reduction of peak dose to about 5 mrem/yr at about 75,000 years, as shown in Figure 8. [Assuming consumption of water due to corrosion of glass in the waste form at the rate of 0.175 grams of water per gram of glass corroded (McGrail, 1995) and replenishment of moisture in the waste form due to percolation through the top of the waste form at the rate of 0.001 cm/yr suggests a water budget deficit in the waste form for the first several thousand years after disposal as shown in Figure 9.]

3.3.5 Intact Concrete Floor: Step-Change to Gravel at 1000 Years

Inclusion of an intact concrete floor at the base of the vault for 1000 years after disposal has no effect on the Concept 1 base case peak dose of 147 mrem/yr at 8600 years. After 1000 years the hydraulic properties of the floor zone are changed to the same base case gravel properties of the waste form in accordance with the assumption that the floor is fractured and has degraded to gravelly rubble.

3.3.6 Concrete Floor: Minimum Conductivity Cutoff - 10^{-20}

The saturated hydraulic conductivity used in the representation of the intact concrete floor is $K_s = 3.75 \times 10^{-10}$ cm/s, from the last line of Table 2. The initial tension assigned to the concrete floor zone was -10 cm. Hence the initial conductivity of the concrete was low (on the order of 10^{-10} cm/s), but the relative conductivity was on the order of about 0.1. After the step change to gravel properties at 1000 years after disposal, moisture leftover

from the concrete floor dissipated and the gravel properties of the degraded concrete floor were similar to those of the gravelly waste form in the base case. At the very low moisture contents realized in the simulated waste form, the relative hydraulic conductivity of the gravel regions is very low (around 10^{-10} or less). But version 2.394gr of PORFLOW enforces a minimum relative conductivity with default value of 10^{-10} . So the simulation with inclusion of the concrete floor was rerun with the minimum $k_r = 10^{-20}$. The results showed no appreciable change from the previous case; the peak calculated dose was 146 mrem/yr at about 8700 years. The noticeable difference between this case and the previous case which had the default minimum $k_r = 10^{-10}$ was in cpu time. The present simulation case required about 21 cpu minutes on the IBM RISC system while the previous case took less than 6 cpu minutes on the same computer.

3.3.7 Lo-QC Sand Filler

Use of Lo-QC sand properties for the filler instead of the Hi-QC sand ("backfill") properties from the base case resulted in a slightly lower peak dose of about 136 mrem/yr at 9,000 years. The lower dose and slightly delayed time of occurrence are believed to be the product of the lower conductivity of the Lo-QC sand (cf. Table 2 and Figure 4).

3.3.8 Sandy Gravel Waste Form

Assignment of sandy gravel hydraulic properties to the canister region results in a peak dose of 145 mrem/yr at 8700 years. This is not significantly different from the Concept 1 base case with gravel canister region. The sandy gravel properties assigned to the canister region for this case are from soil sample 241-AP-1g, which is the same soil as the 241-AP-1 sample but with 38% gravel by volume. At the residual volumetric moisture content of $\theta = 0.021$, the relative hydraulic conductivity for this sandy gravel is $k_r = 6 \times 10^{-9}$ and hence the results of this simulation case are not influenced by the default minimum relative conductivity of 10^{-10} .

Figure 10 shows relative hydraulic conductivity characteristic curves for five additional Hanford sandy gravel soil samples as well as for the gravel sample represented in Table 2. These five additional sandy gravel soils have gravel content ranging from 42% up to 55% by volume. The plots in Figure 9 suggest that the relative conductivity curves tend to converge at high tensions. The discrimination between the sandy gravels is determined largely by saturated hydraulic conductivity which varies over about a couple orders of magnitude. But the relative conductivities shown in Figure 10 vary over about ten orders of magnitude within a couple percent change in volumetric moisture content near the residual volumetric moisture content. This means that large fluctuations in hydraulic conductivity of any of these materials can be expected with only slight changes in calculated moisture content in the simulation model. Hence the model is not expected to be sensitive to changes in properties of the sandy gravel or gravel canister region, but rather to changes in moisture content of the canister region.

3.3.9 Side Influx: 100% Return of Diverted Moisture ($a=0.1$)

Under the assumption that the downdip end of the capillary barrier is above the elevation of the floor of the vault, it might be possible for moisture diverted from the capillary barrier to diffuse back toward and into the vault and waste form. This seems particularly germane to Concept 2 in which each row of storage bays has its own capillary barrier and for which the mean return distance is relatively small compared to Concept 1. For the present simulation case, the Concept 1 base case is used with postulated return of 100% of the moisture diverted by a 90% effective capillary barrier ($a=0.1$). The total volume of returning moisture per unit time is $(1-a)q$ times the area of the top of the model (area = 1.05 m^2). The returning moisture is uniformly distributed over the 9 m height from the bottom of the canister region to the top of the model (top of the vault) on the downdip (right) side of the model. The result is a peak dose of about 198 mrem/yr at 31,000 years.

3.3.10 Side Influx: 50% Return of Diverted Moisture ($a=0.1$)

Repeating the side influx scenario immediately above but with assumed 50% of diverted moisture returning results in a peak dose of about 106 mrem/yr at about 35,000 years. Results of the three cases with the 90% effective capillary barrier ($a=0.1$) and 100%, 50%, and 0% return are summarized in Figure 11.

3.3.11 Capillary Barrier: $a=0.1$ with Minimum $k_r = 10^{-20}$

The default PORFLOW threshold for minimum relative conductivity was shown to not be an important factor in the base case scenarios without the effect of a capillary barrier. With decreasing amount of moisture available to the waste form due to an effective capillary barrier, it seems that the conductivity cutoff might become more important to the accuracy of the simulation results. The present case revisits the base case with a 90% effective capillary barrier ($a=0.1$) and minimum relative hydraulic conductivity set at 10^{-20} . The result is a peak dose of about 23 mrem/yr at about 39,000 years compared to a peak of about 32 mrem/yr for the same case with minimum $k_r = 10^{-10}$.

3.3.12 Moisture Withdrawal: $a=0.1$ and Minimum $k_r = 10^{-20}$

An extension of the case immediately above including the effect of moisture withdrawal due to consumption of water during glass corrosion at the rate of 0.175 grams of water per gram of glass dissolved results in a further reduction of peak drinking dose to about 17 mrem/yr at about 40,000 years. A summary of the effects of moisture withdrawal and/or the conductivity threshold in the presence of a 90% effective capillary barrier is shown in Figure 12.

3.3.13 Sandy/Gravel Waste Form: Minimum $k_r = 10^{-20}$

Further variations of the waste form properties with inclusion of the minimum relative hydraulic conductivity set to 10^{-20} all resulted in the same peak dose of about 148 mrem/yr at about 8800 years. The simulation cases included the following variations of the base case hydraulic property assignments:

Waste Form	Filler
Sandy Gravel	Hi-Qc Sand
Lo-QC Sand	Hi-QC Sand
Hi-QC Sand	Hi-QC Sand
Hi-QC Sand	Lo-QC Sand
Lo-QC Sand	Lo-QC Sand
Sandy Gravel	Gravel

The volumetric moisture content of the waste form is effectively at the residual θ_r for each of the simulations. At that low moisture content, the conductivity of the waste form is so low that the release of contaminants from the waste form is likely dominated by diffusion.

3.3.14 Effect of Initial Conditions: Minimum $k_r = 10^{-20}$

Each of the simulations is started from an initial steady state flow field such as shown in Figure 6. For cases with material property variations like those shown immediately above, each material that is different from materials used in the steady state is re-assigned an appropriate initial pressure head based on the assumed recharge and an assumed unit gradient. In the base case variation above with sandy gravel waste form and gravel filler, initial pressure heads of both of those materials were varied from -1000 cm to -1 cm. That range of initial pressure heads corresponds to air-dry at -1000 cm up to near saturation at -1 cm for the assumed sandy gravel waste form. The gravel volumetric moisture content ranges from residual at -1000 cm up to about 6% at -1 cm. With the variations in initial moisture content, all cases resulted in a peak dose of about 148 mrem/yr between 8800 and 9000 years after time of disposal.

A final related case with initial pressure head of $\psi = -1000$ cm in the sandy gravel waste form resulted in the same peak dose of about 148 mrem/yr at about 9000 years, even with the head fixed (held constant) in the waste form at the uniform initial value for the duration of the simulation. The fixed uniform head everywhere in the waste form implies zero pressure gradient and zero velocity everywhere in the waste form and hence no advection of contaminants within the waste form. Obtaining the same dose as when advection is not disabled in the waste form implies that transport in the waste form is indeed diffusion dominated.

3.3.15 Tc-99 Transport Properties in the Waste Form

The peak drinking water doses detailed in the foregoing cases are largely due to Tc-99 in the LLW (Rawlins et al, 1994). Since transport within the waste

form is diffusion controlled, dose sensitivity to changes in the diffusion coefficient for Tc-99 was investigated. The base value of the diffusion coefficient for all species in all materials is $2.5 \times 10^{-5} \text{ cm}^2/\text{s}$. Variation of the diffusion coefficient for Tc-99 in a sandy gravel waste form (canister region) by two orders of magnitude about the base value resulted in no change to the peak dose of about 148 mrem/yr at about 8900 years. Variations of the diffusion coefficient with simultaneous variations in the moisture content of the sandy gravel waste form also obtained no change in the simulated peak dose.

3.3.16 Well Intercept Factor

Contaminant concentrations in moisture moving downward through the vadose zone are diluted substantially upon entering the faster moving horizontal groundwater flux of the unconfined aquifer. Water taken from the postulated well 100 meters downgradient from the disposal facility will have been drawn from all directions around the open interval of the well casing (due to the "cone of depression" created by pumping). The extent of the cone of depression depends on the pumping rate and the aquifer transmissivity. Dilution at the well depends on the extent of the cone of depression and the areal and vertical extent to which contaminant is spread in the aquifer. This is in turn related to the physical extent and orientation of the disposal facility. The net effect of these influences is included in an empirical factor referred to as the "Well Intercept Factor", which is the ratio of contaminant concentration in water drawn from the well to contaminant concentration in moisture seeping through the vadose zone (Rawlins et al., 1994).

The well intercept factor used for the Grout PA (Kincaid et al., 1995) was taken to be 0.01. Rescaling the well intercept factor for change in facility dimensions gave a value of 0.006 for the central analysis case described by Rawlins et al. (1994). That value has been used here and is reflected in all of the dose results presented herein to this point. Rescaling the well intercept factor for use here in accordance with facility dimensions given by Eiholzer (1995) gives a value of 0.017 for Concept 1 and a value of 0.007 for Concept 2. The effect of the well intercept factor on dose results is linear. The effect of scaling the well intercept factor can be obtained simply by scaling the doses by the same amount.

3.3.17 Inventory

The LLW inventory used for all of the simulation cases reported herein to this point is the same as used by Rawlins et al. (1994). A new evaluation of the inventory has recently been prepared by Schmittroth (1995). Revisitation of the dose calculation for the Concept 1 base case with the re-evaluated inventory and with the well intercept factor rescaled to the value of 0.017 for Concept 1 as described above obtains a peak dose of about 438 mrem/yr at about 8600 years as shown in Figure 13.

3.3.18 Summary of Dose Results

The base case simulation with the unit cell model serves to benchmark the accuracy and computational efficiency of the unit cell approach against the full facility models. The base case also provides a benchmark dose against which to compare effects of model variations. A summary of comparisons of peak doses from the other simulation cases described above to the peak dose from the base case is contained in Table 4. Letting p_0 denote the peak dose of 147 mrem/yr from the base case and letting p_i denote the peak dose for the i^{th} case above ($i = I$ through XVI), the percent difference of the i^{th} case from the base case in the last column of Table 4 below is $(1 - p_i/p_0) \times 100\%$. A positive value indicates a decrease in peak dose and a negative number indicates an increase in peak dose. From the last column in Table 4 it appears that two of the most important parameters among those varied for this work are capillary barrier effectiveness and the well intercept factor. Capillary barrier effectiveness is important in that a 99% effective capillary barrier reduces the peak dose by about 97% and prolongs the arrival time of the peak dose by almost a factor of nine (from about 8600 years to about 75,000 years), assuming no return of diverted moisture to the waste form. The well intercept factor is important in that the dose at any point in time is directly proportional to the well intercept factor.

Table 4. Comparison of Peak Doses.

Simulation Case	Peak Dose (mrem/yr)	Change from Base Case
Section 3.3.1 Concept 1: 10 cm Inter-Canister Spacing	147	--
Section 3.3.2 Concept 2: 35 cm Inter-Canister Spacing	112	24%
Section 3.3.3 Capillary Barrier: $\alpha=0.1$	32	78%
Section 3.3.4 Capillary Barrier: $\alpha=0.01$	5	97%
Section 3.3.5 Intact Concrete Floor: Step-Change to Gravel at 1000 Years	147	0
Section 3.3.6 Concrete Floor: Minimum Conductivity Cutoff - 10^{-20}	146	0
Section 3.3.7 Lo-QC Sand Filler	136	7%
Section 3.3.8 Sandy Gravel Waste Form	145	1%
Section 3.3.9 Side Influx: 100% Return of Diverted Moisture ($\alpha=0.1$)	198	-35%
Section 3.3.10 Side Influx: 50% Return of Diverted Moisture ($\alpha=0.1$)	106	28%
Section 3.3.11 Capillary Barrier: $\alpha=0.1$ with Minimum $K_r = 10^{-20}$	23	84%
Section 3.3.12 Moisture Withdrawal: $\alpha=0.1$ and Minimum $K_r = 10^{-20}$	17	88%
Section 3.3.13 Sandy/Gravel Waste Form: Minimum $K_r = 10^{-20}$	148	0
Section 3.3.14 Effect of Initial Conditions: Minimum $K_r = 10^{-20}$	148	0
Section 3.3.15 Tc-99 Transport Properties in the Waste Form	148	0
Section 3.3.16 Well Intercept Factor	416	-183%
Section 3.3.17 Inventory	438	-198%

4.0 SUMMARY AND CONCLUSIONS

This report focuses on development of a unit cell model used in analysis of some design options for a vitrified low-level waste (LLW) disposal facility. The unit cell modeling approach is also likely to be useful in the upcoming Interim Performance Assessment for the facility.

Two present disposal facility concepts differ substantially in the length of a capillary barrier proposed to limit effective recharge through the top of the facility. A capillary barrier is a layer of fine soil overlying a layer of coarser soil, and generally sloped away from a central point to promote drainage. Capillary barriers are analyzed independently for this work; the effect of a capillary barrier is treated as a parameter in the unit cell model. The unit cell model extends vertically from the top of the facility walls to the water table of the uppermost aquifer system and provides comparative results for various simulation scenarios in terms of total radiation dose from drinking water.

Analytical models (e.g. Ross, 1990; Morel-Seytoux, 1994; Stormont, 1995) provide formulae from which to estimate effective length of a capillary barrier. With an assumed recharge rate of 0.1 cm/yr and assumption that the fine layer of the barrier is composed of common local material such as the fine soil from Sample 241-AP-1 taken from the upper Hanford formation at the AP Tank Farm in the 200 East Area, the analytical models give estimates of effective length on the order of kilometers for a two-sided barrier that is peaked at the center. Analytical criteria for required thickness of the fine layer of a capillary barrier suggest necessary thickness on the order of a meter or less for common local material.

Field-scale observations of a capillary barrier in East Wenatchee, Washington for about a two year period showed favorable comparison to a traditional resistive barrier (Khire et al., 1994). In comparison of the two 30 meter long experimental barriers, the resistive barrier allowed twice the rate of seepage through the barrier as did the capillary barrier of the same length. The experiment also showed that the capillary barrier was effective with a relatively thin (15 cm thick) fine layer of soil and no slope to promote drainage.

Finite element based numerical simulations of capillary barrier performance by Nichols and Meyer (1995) suggest near 100% effectiveness for a Hi-QC barrier of length 28 meters under recharge of 32 cm/yr (about twice the local average annual precipitation). Their results also verify that capillary barrier performance can be highly sensitive to selection of materials; equivalently, capillary barrier performance is highly sensitive to the recharge rate in that barrier performance declines as the recharge rate approaches the point at which the conductivity of the fine material in the barrier is equal to the conductivity of the coarse material in the barrier.

Finite difference based simulations of capillary barrier performance reported here extend the work of Nichols and Meyer (1995) to longer barrier lengths and lower recharge rates. The new simulation model was successfully benchmarked against the Nichols and Meyer (1995) model for some Hi-QC barrier cases at the

high recharge rate of 32 cm/yr. The exact finite element representation of a sloping interface and the stair-stepped finite difference representation provided comparable results for the benchmark cases. Further simulations suggest near 100% effectiveness for Hi-QC barriers of total (two-sided) length up to 800 meters with slopes from 2.5% to 20% and recharge rates from 32 cm/yr down to 0.01 cm/yr. Some limited variation of material properties at the recharge rate of 0.01 cm/yr obtained no evidence of variability of capillary barrier performance.

Results of analytical, experimental and numerical work reviewed and summarized here suggest that design of a capillary barrier which can reduce a recharge rate of 0.1 cm/yr by one or even two orders of magnitude seems feasible for both Concept 1 and Concept 2. Longevity and continued performance of a capillary barrier on a geologic time scale remain to be evaluated. Collapse of intentional voids in the engineered disposal facility could likely lead to subsidence of the overlying barriers which might lead to degradation of performance.

The unit cell model for predicting performance of a LLW glass disposal facility is based on the performance of a single one of the proposed 6804 canisters to be emplaced in the facility. Effect of a capillary barrier over the system is treated as a parameter in the recharge boundary condition at the top of the model. Simulation of a base case with the unit cell model obtains a peak drinking water dose of about 147 mrem/yr at about 8600 years, which is within about 1% of the predicted peak dose for the same base case simulated with a full facility model. The unit cell model runs the base case in about 5 minutes of computer time while the full facility model takes from 12 to 15 hours of computer time for the same base case. Computational accuracy and efficiency of the unit cell approach make the unit cell approach desirable for further work in support of facility design analyses and the IPA.

The present base case for Concept 1 and Concept 2 (Eiholzer 1995) with the unit cell model differ only by the thickness of the intercanister filler material. Increasing the intercanister spacing from 10 cm under Concept 1 to 35 cm under Concept 2 decreases peak drinking dose by about 24% of the Concept 1 base case peak dose. This is due to lowered moisture content in the filler with the greater intercanister spacing.

Imposition of a 90% effective capillary barrier reduces the effective recharge rate by an order of magnitude and reduces the peak radiation dose from drinking water by about 78% of the base case peak dose. Assuming that 100% of the moisture diverted by a 90% effective capillary barrier returns as lateral influx through the intercanister filler material can increase peak drinking dose by about 35% of the base case peak dose. The postulated moisture return scenarios considered for this work might be aphysical in that 100% return or even 50% return might be an exaggeration of expected lateral return of moisture diverted by a capillary barrier. Those scenarios suggest however that lateral return of moisture can be important and therefore the amount of lateral return should be quantified and included in further modeling efforts.

Assuming consumption of water due to glass corrosion at the rate of 0.175 grams of water per gram of glass corroded reduces the peak dose a few percent.

Imposition of a 99% effective capillary barrier reduces the effective recharge rate by two orders of magnitude and reduces peak dose by about 97%. Replenishment of water under assumption of a 99% effective capillary barrier and consumption of water due to glass corrosion can lead to a water balance deficit in the waste form for the first several thousand years after disposal.

Transport of contaminants through the vadose zone from the bottom of the facility to the water table is dominated by advection in the model (i.e., dissolved contaminants are transported by the diffusion of moisture). Variations of material properties and state variables in the zone of the model representing the waste form shows that transport of dissolved contaminants in the modeled waste form is largely controlled by diffusion in the moisture.

Re-evaluation of the LLW inventory by Schmittroth (1995) suggests a few percent increase in peak base case drinking dose. This is due largely to inclusion of ⁷⁹Se in the inventory.

In all cases, simulated drinking water dose at any point in time is proportional to the well intercept factor. Substantiation of the use of the well intercept factor could be investigated using numerical simulations of groundwater flow and transport including effects of facility size and orientation, shedding of infiltrating moisture from a capillary barrier, media heterogeneity, and pumping rate at the well from which drinking water is derived.

Another factor which potentially can affect peak drinking doses and arrival time of peak doses is depth of the vadose zone. For the present work the depth of the vadose zone from ground surface to the water table of the uppermost aquifer system is assumed to be about 80 meters. This is consistent with modeling performed for the Grout PA (Kincaid et al., 1995) and with the central analysis case reported by Rawlins et al. (1994). However, in a recent review of vadose zone sampling and hydrologic properties of vadose zone materials in support of the upcoming IPA, Khaleel and Freeman (1995) suggest that depth of the water table below land surface is between 100 meters and 120 meters at the Grout Site and surrounding sites at the 200 East and 200 West Areas. Increased depth to the water table is expected to lengthen arrival time and decrease peak dose.

5.0 REFERENCES

- DOE, 1988, "Radioactive Waste Management," DOE Order 5820.2A, U.S. Department of Energy, Washington D.C.
- Ecology, EPA and DOE, 1994, "Hanford Federal Facility Agreement and Consent Order," document available from Washington State Department of Ecology, U.S. Environmental Protection Agency, and U.S. Department of Energy.
- Eiholzer, C. R., 1995, "Disposal Facility Data for the Interim Performance Assessment," WHC-SD-WM-RPT-159, Rev. 0, Westinghouse Hanford Company, Richland, Washington.
- Khaleel, R. and E. J. Freeman, 1995, "A Compilation of Hydrologic Properties for Low-Level Glass Waste Disposal Facility Performance Assessment," WHC-SD-WM-RPT-0165, Rev. 0, Westinghouse Hanford Company, Richland, Washington.
- Khaleel, R. and T. LeGore, 1990, "Effects of Varying Recharge on Radionuclide Flux Rates to the Water Table at a Low-Level Solid Waste Burial Site," WHC-SA-0699-FP, Westinghouse Hanford Company, Richland, Washington.
- Khire, M. V., C. H. Benson, P. J. Bosscher and R. J. Pliska, 1994, "Field-Scale Comparison of Capillary and Resistive Landfill Covers in an Arid Climate," Proceedings of the Fourteenth Annual AGU Hydrology Days held 4/5-4/8/95 in Fort Collins, Colorado.
- Kincaid, C. T., J. W. Shade, G. A. Whyatt, M. G. Piepho, K. Rhoads, J. A. Voogd, J. H. Westsik, Jr., M. D. Freshley, K. A. Blanchard and B. G. Lauzon, 1995, "Performance Assessment of Grouted Double-Shell Tank Wastes Disposal at Hanford," WHC-SD-WM-EE-004, Rev. 1, Westinghouse Hanford Company, Richland Washington.
- Kline, N. W., 1994, "Certification of Version 1.2 of the PORFLO-3 Computer Code for the WHC Scientific and Engineering Computational Center," WHC-SD-WM-CSWD-069 Rev. 0, Westinghouse Hanford Company, Richland, Washington.
- Kline, N. W. and R. Khaleel, 1995, "Effect of Moisture-Dependent Anisotropy and Enhanced Recharge Around Underground Storage Tanks," Proceedings of the ANS International Conference on Mathematics and Computations, Reactor Physics, and Environmental Analyses held 4/30-5/4/95 in Portland, Oregon; also WHC-SA-2680-FP.
- McCord, J. T., D. B. Stephens and J. L. Wilson, 1991, "Hysteresis and State-Dependent Anisotropy in Modelling Unsaturated Hillslope Hydrologic Processes," Water Resources Research, Vol. 27, No. 7, pp. 1501-1518.
- McGrail, B. P., 1995, "Water Mass Balance for Glass Corrosion," Correspondence from Pete McGrail to John Rawlins dated 8/8/95.

- Morel-Seytoux, H. J., 1994, "Steady-State Effectiveness of a Capillary Barrier on a Sloping Interface," Proceedings of the Fourteenth Annual AGU Hydrology Days held 4/5-4/8/94 in Fort Collins, Colorado.
- Myers, D. R. and D. A. Duranceau, 1994, "Prototype Hanford Surface Barrier: Design Basis Document," BHI-00007, Rev. 00, Bechtel Hanford, Inc., Richland, Washington.
- Nichols, W. E. and P. D. Meyer, 1995, "Multidimensional Water Flow in a Low-Level Waste Isolation Barrier," accepted for Publication in Groundwater.
- Piepho, M. G., W. H. Sutherland and P. D. Rittman, 1994, "The Grout/Glass Performance Assessment Code System (GPACS) with Verification and Benchmarking," WHC-SD-WM-UM-019, Rev. 0, Westinghouse Hanford Company, Richland, Washington.
- Piepho, M. G., 1995, "Preliminary Results of Concept 1 & 2 Designs," Correspondence to F. Mann, C. Eiholzer and D. Mitchell dated 7/11/95, Daniel B. Stephens & Associates, Inc., Richland Washington.
- Rawlins, J. A., R. A. Karnesky, R. Khaleel, A. H. Lu, F. M. Mann, B. P. McGrail, W. J. McMahon, M. G. Piepho, P. D. Rittman and F. A. Schmittroth, 1994, "Impacts of Disposal System Design Options on Low-Level Glass Waste Disposal System Performance," WHC-EP-0810, Rev. 0, Westinghouse Hanford Company, Richland, Washington.
- Rockhold, M. L., M. J. Fayer, C. T. Kincaid, and G. W. Gee, 1995, "Estimate of the Natural Groundwater Recharge for the Performance Assessment of a Low-Level Waste Disposal Facility at the Hanford Site," PNL-10508, Pacific Northwest Laboratory, Richland, Washington.
- Ross, B., 1990, "The Diversion Capacity of Capillary Barriers," Water Resources Research, Vol. 26, No. 10, pp. 2625-2629.
- Ross, B., 1991, "Reply," Water Resources Research, Vol. 27, No. 8, p. 2157.
- Runchal, A. K., B. Sagar and N. W. Kline, 1992, "PORFLO-3: A Mathematical Model for Fluid Flow, Heat, and Mass Transport in Variably Saturated Geologic Media. Users Manual, Version 1.2," WHC-EP-0385, Westinghouse Hanford Company, Richland, Washington.
- Schmittroth, F. A., 1995, "Inventories for the Low-Level Waste Interim Performance Assessment," WHC-SD-WM-RPT-165, Westinghouse Hanford Company, Richland, Washington.
- Smoot, J. L., J. E. Szecsody, B. Sagar, G. W. Gee and C. T. Kincaid, 1989, "Simulations of Infiltration of Meteoric Water and Contaminant Plume Movement in the Vadose Zone at Single-Shell Tank 241-T-106 at the Hanford Site," WHC-EP-0332, Westinghouse Hanford Company, Richland, Washington.

- Stephens, D. B. and S. Heermann, 1988, "Dependence of Anisotropy on Saturation in a Stratified Sand," Water Resources Research, Vol. 24, No. 5, pp. 770-778.
- Steenhujs, T. S., J.-Yves Parlange and K.-J. Samuel Kung, 1991, "Comment on 'The Diversion Capacity of Capillary Barriers' by Benjamin Ross," Water Resources Research, Vol. 27, No. 8, pp. 2155-2156.
- Stormont, J. C., 1995, "The Effect of Constant Anisotropy on Capillary Barrier Performance," Water Resources Research, Vol. 31, No. 3, pp. 783-785.
- van Genuchten, M. Th., 1980, "A Closed-Form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils," Soil Sci. Soc. Am. J., Vol. 44, pp. 892-898.
- Yeh, T.-C. J., L. W. Gelhar and A. L. Gutjahr, 1985a, "Stochastic Analysis of Unsaturated Flow in Heterogeneous Soils, 1. Statistically Isotropic Media," Water Resources Research, Vol. 21, No. 4, pp. 447-456.
- Yeh, T.-C. J., L. W. Gelhar and A. L. Gutjahr, 1985b, "Stochastic Analysis of Unsaturated Flow in Heterogeneous Soils, 2. Statistically Anisotropic Media with Variable α ," Water Resources Research, Vol. 21, No. 4, pp. 457-464.
- Yeh, T.-C. J., L. W. Gelhar and A. L. Gutjahr, 1985c, "Stochastic Analysis of Unsaturated Flow in Heterogeneous Soils, 3. Observations and Applications," Water Resources Research, Vol. 21, No. 4, pp. 465-471.

Figure 1. Schematic Diagram of Capillary Barrier Model.

Figure 2. Steady-State Effective Saturation for Hi-QC Capillary Barrier with 5% Slope under 0.1 cm/yr Recharge.

Figure 3. Steady-State Effective Saturation for Hi-QC Capillary Barrier with 20% Slope under 0.1 cm/yr Recharge.

Figure 4. Characteristic Curves for Sand and Gravel Barrier Materials.

Figure 5. Schematic Drawing of Unit Cell Model.

Figure 6. Steady-State Saturation Distribution with Streamlines.

Figure 7. Comparison of Peak Doses from Concept 1 and Concept 2.

Figure 8. Reduction of Drinking Doses due to Capillary Barrier Effectiveness.

Figure 9. Bulk Rates of Change of Volumetric Moisture Content in the Waste Form.

Figure 10. Characteristic Curves for Gravel and Five Sandy Gravel Sediment Samples.

Figure 11. Decrease in Dose with Decrease in Return of Moisture Diverted by a Capillary Barrier.

Figure 12. Effect of Moisture Withdrawal due to Corrosion.

Figure 13. Principal Contributors to Base Case Drinking Water Dose.

APPENDIX A

Referenced Correspondence

Piepho 1995 Page A-2

McGrail 1995 Page A-32

Date: July 11, 1995

To: F. Mann, C. Eiholzer, D. Mitchell

From: M. Piepho *MGP*

Subject: Preliminary Results of Concept 1 & 2 Designs

Please find attached the graphs of drinking-water doses, steady-state moisture contents, and relative concentrations at representative times for four Concept 1 cases and five Concept 2 cases. Due to the larger gravel wedge used in Concept 1, the Concept 1 design produces much lower doses (about a factor of five) than Concept 2's design. The bottom line of these simulations is that the gravel wedge is very important and should be designed in an optimum manner.

The nine simulated cases are briefly described here.

Case Name

Lfbase1-6 - Base case for Concept 1; release rate of glass is based on a corrosion rate of $1.E-5$ cm/yr and a glass radius of 0.25 cm, i.e., 25,000-yr glass. The concrete is assumed to be fractured and the glass-sulfur polymer cement canisters are assumed to be completely fractured such that each glass marble is exposed to water. The recharge below the Hanford barrier is assumed to be 0.1 cm/yr. The canisters are 2 m x 2 m x 8 m, with 95% fill of glass cullet/sulfur-polymer cement, and the top 5% being a void or air space.

- Maximum dose of about 18 mrem/yr.

Lfbase2-6 - Base case for Concept 2.

- Maximum dose of about 100 mrem/yr.

Lfbase1-7 - Same as base case for Concept 1 except that recharge is increased to 0.2 cm/yr.

- Maximum dose of about 20 mrem/yr.

Lfbase2-7 - Same as base case for Concept 2 except that recharge is increased to 0.5 cm/yr.

- Maximum dose of about 120 mrem/yr.

Lfbase1-8 - Same as Concept 1 base case, except that no gravel wedge is used.

- Maximum dose of about 145 mrem/yr.

Lfbase2-8 - Same as Concept 2 base case, except that no gravel wedge is used.

- Maximum dose about 145 mrem/yr.

Lfbase2-9 - Same as Concept 2 base case, except that an improved gravel wedge, which runs vertically along the sides of the vault is used.

- Maximum dose of about 70 mrem/yr.

Lfbase2-10 - Same as Concept 2 base case, except that one piece of gravel wedge has subsided 30 cm due to one canister's top air space being filled by backfill soil.

- Maximum dose of about 100 mrem/yr.

case5-3 - Same as Concept 1 base case, except that glass surface area exposed to water is reduced to 35 times the surface area of the glass/SPC monolith in each canister. This results in a glass that lasts about 375,000 years instead of 25,000 years.

- Maximum dose is about 5 mrem/yr after 100,000 years of disposal.

Again, the main conclusion of these preliminary results is that the gravel wedge design is very important for peak doses. Also, the glass release rate is important as shown by case5-3. Recharge is not as important as either the gravel wedge or glass release rate for these cases. Basically, the gravel wedge takes away most of the higher recharge effects.

Concept 1 Base Case

Concept I Base Case

Concept 1
- No Gravel wedge

(2D) || Print || 9 Jul 1995 || Lfbase1-8.plt || Lfbase1-8;no gravel wedge,cracked concrete,1cmrecharge, degraded concrete

(PORFLOW-SDVERSION 2.35)
(Last Modified on 10/18/92)
(Run Made by ACRU-GEN)
(On 01/01/1992 at 00:12)
Z = 0.00000E+00

Concept 1
- No Gravel Wedge

(2D) || Print || 9 Jul 1995 || Lfbase1-8.plt || Lfbase1-8;no gravel wedge,cracked concrete,1cmrecharge, degraded concrete

(PORFLOW-SD VERSION 2.5F)
(Last Modified on 10/18/92)
Run Made by ACRI-GEN
(On 01/31/1992 at 00:12)
Z = 0.00000E+00

Concept 1 Base Case

Concept 1

~ Recharge = 0.2 cm/yr

(2D) || Print || 9 Jul 1995 || Lfbase1-7.plt || Lfbase1-7:cracked concrete,2cmrecharge, degraded concrete32 sources,

(PORTFLOW-3D VERSION 2.36)
(Last Modified on 10/11/92)
(Run Made by ACRI-GEN)
(On 01/31/1992 at 00:12)
Z = 0.00000E+00

Concept 1

- Recharge = 0.2 cm/yr

(2D) || Print || 9 Jul 1995 || Lfbase1-7.plt || Lfbase1-7;cracked concrete,2cmrecharge, degraded concrete32 sources,

(PORFLOW-3D VERSION 2.35)
(Last Modified on 10/12/92)
(Run Made by ACRI-GEN)
(On 01/31/1992 at 00:12)
Z = 0.00000E+00

Concept 2 Base Case

Concept 2 Base Case

(2D) || Print || 8 Jul 1995 || Lfbase2-6.plt || Lfbase2-6;concept2,cracked concrete,1cmrecharge, degraded concrete32 so

(PORFLOW-SDVERSION 2.39)
(Last Modified on 10/18/92)
(Run Made by ACRI-GEN)
(On 01/31/1992 at 00:12)
Z = 0.00000E+00

5000 y/a

c 0.5Kyr3

Concept 2 - Small Gravel Subsidence Failure

Concept 2

- Small Gravel Subsidence Failure

(2D) || Print || 9 Jul 1995 || Lfbase2-10.plt || Lfbase2-10;concept2,gravel failure,1cmrecharge,degraded concrete8 source

(FORFLOW-3DVERSION 2.35)
(Last Modified on 10/18/92)
(Run Made by ACRU-GEN)
(On 01/31/95 at 10:12)
Z = 0.00000E+00

Concept 2
- Small Gravel Subsidence Failure

(2D) || Print || 9 Jul 1995 || Lfbase2-10.plt || Lfbase2-10.concept2.gravel failure.1cmrecharge, degraded concrete8 source

(PDFLOW-3D VERSION 2.39)
(Last Modified on 10/18/92)
(Run Made by ADRI-GEN)
(On 01/31/1992 at 00:12)
Z = 0.00000E+00

Concept 2 Base Case

(2D) || Print || 9 Jul 1995 || Lfbase2-6.plt || Lfbase2-6,concept2,cracked concrete.1cmrecharge, degraded concrete32 so

(PCRFLOW-3DVERSION 2.36)
Last Modified on 10/18/92
(Run Made by ACR1-GEN)
(On 01/31/1992 at 00:12)
Z = 0.00000E+00

Concept 2
- No Gravel Wedge

(2D) || Print || 9 Jul 1995 || Lfbase2-8.plt || Lfbase2-8,concept2,no gravel wedge,1cmrecharge,degraded concrete8 sour

(PORFLOW-SD VERSION 2.25)
(Last Modified on 10/18/92)
(Run Made by ACR1-GEN)
(On 01/21/1992 at 00:12)
Z = 0.00000E+00

Concept 2
- No Gravel Wedge

(2D) || Print || 9 Jul 1995 || Lfbase2-8.plt || Lfbase2-8;concept2,no gravel wedge,1cmrecharge, degraded concrete8 sour

(PCRFLOW-3DVERSION 2.39)
(Last Modified on 10/18/92)
(Run Made by ACR1-GEN)
(On 01/31/1992 at 00:12)
Z = 0.00000E+00

(2D) || Print || 9 Jul 1995 || Lfbase2-9.plt || Lfbase2-9,concept2,improved gravel wedge,1cmrecharge, degraded concrete

Concept 2

- Improved Gravel Wedge

(2D) || Print || 9 Jul 1995 || Lfbase2-9.plt || Lfbase2-9;concept2,improved gravel wedge,1cmrecharge, degraded concrete

(PCFLOW-3DVERSION 2.35)
(Last Modified on 10/7/92)
(Run Made by ACRI-GEN)
(On 01/31/1992 at 00:12)
Z = 0.00000E+00

(2D) || Print || 10 Jul 1995 || Lfbase2-9.plt || Lfbase2-9;concept2,improved gravel wedge.1cmrecharge, degraded concrete

(PORFLOW-3DVERSION 2.34)
(Last Modified on 10/13/92)
(Run Made by ACRU-GEN)
(On 01/31/1992 at 00:12)
Z = 0.00000E+00

Concept 1 Base Case
- 25,000 yr glass release
- recharge = 0.1 cm/yr

(2D) || Print || 10 Jul 1995 || Lfbase1-6.plt ||

Concept 1
- No Gravel Wedge

(2D) || Print || 10 Jul 1995 || Lfbase1-8.plt ||

Concept 1
- recharge = 0.2 cm/yr

(2D) || Print || 10 Jul 1995 || Lfbase1-7.plt ||

Preliminary Drinking Dose (mrem/yr) based on old dose model

Concept 1

Source Term with Surface Area
= 35 x Monolith SA

(2D) || Print || 11 Jul 1995 || case5-3.plt ||

Concept 1
Source Term with Surface Area
= 35 x Monolith SA

(2D) || Print || 11 Jul 1995 || case5-3.plt ||

Concept 2 Base Case
- 25,000 yr glass (0.25 cm radius)
- recharge = 0.1 cm/yr

(2D) || Print || 10 Jul 1995 || Lfbase2-6.plt ||

Concept 2
- No Gravel Wedge

(2D) || Print || 10 Jul 1995 || Lfbase2-8.plt ||

Concept 2
- Improved Gravel Wedge

(2D) || Print || 10 Jul 1995 || Lfbase2-9.plt ||

Concept 2
- small Gravel Subsidence Failure

(2D) || Print || 10 Jul 1995 || Lfbase2-10.plt ||

Concept 2
- recharge = 0.5 cm/yr

(2D) || Print || 10 Jul 1995 || Lfbase2-7.plt ||

DON'T SAY IT--Write It!

Date: August 8, 1995

To: John Rawlins

From: Pete McGrail 5-2015

Subject: Water Mass Balance for Glass Corrosion

A calculation was performed to estimate whether there is sufficient water at a recharge rate of 0.1 cm/y to react with the LLW glass and therefore solubilize the ^{99}Tc inventory.

Calculation of Water Consumption Rate

Assuming 210,000 m³ of LLW glass are produced into spheres that are 1 cm in diameter, the total number of marbles to be produced, N , is

$$N = 210,000 \cdot \frac{3}{4\pi(0.005)^3} = 4 \times 10^{11} \quad (1)$$

The total initial surface area is therefore given by

$$A = 4 \times 10^{11} [4\pi(0.005)^2] = 1.26 \times 10^8 \text{ m}^2 \quad (2)$$

If we assume that the glass corrodes at a fixed rate of $10^{-3} \text{ g/m}^2 \cdot \text{d}$, it is possible to calculate the rate of water consumption by the corrosion reaction if the assemblage of alteration phases formed from the corrosion reaction is known. For this, the EQ3/6 code was used to calculate an assemblage of alteration minerals for a PNL glass formulation, LD6-5510. The details of the calculation results will not be discussed in this note, however the mass of water consumed from the reaction of 0.5 mol of glass was 5.6 g, so an estimate of the water consumption from the hydrolysis of the glass is about 11.2 g_w/mol-glass or 0.175 g_w/g-glass. Assuming that all the glass surface is exposed and is in contact with water (worst case scenario), the total mass of water consumed per year is

$$\dot{m}_w = \frac{10^{-3} \text{ g}}{\text{m}^2 \cdot \text{d}} \times 365 \frac{\text{d}}{\text{y}} \times 0.175 \frac{\text{g}_w}{\text{g-glass}} \times 1.26 \times 10^8 \text{ m}^2 = 8 \times 10^6 \frac{\text{g}_w}{\text{y}} \quad (3)$$

Calculation of Water Mass Flow Rate

Figure 1 is schematic of the geometry assumed for the waste vault. If it assumed that the vault is 10 m thick, then the cross sectional area of the vault, A_c , can be estimated from

$$A_c \times 10\text{m} = \frac{210,000}{(1-\varepsilon)} \quad (4)$$

where ε = porosity of glass bed in the vault. Assuming a porosity of 0.4, the cross-sectional area of the vault is $3.5 \times 10^4 \text{ m}^2$. The mass flow rate of water through the vault can be calculated if we assume hydraulic steady-state so that the 0.1 cm/y recharge rate is equal to the Darcy fluid velocity, V_D . The water flow through the vault region is therefore given by

Figure 1. Schematic of Waste Disposal Vault

$$\dot{m}_w = \theta \rho V_D A_c = 0.15 \times 10^6 \times 0.001 \times 3.5 \times 10^4 = 5.25 \times 10^6 \frac{\text{g}}{\text{y}} \quad (5)$$

where

θ = saturation index
 ρ = density of water, g/m³.

In Equation (5), it has been assumed that the saturation index in the vault is 15%.

CONCLUSION

Given that there is uncertainty in both the calculation of the water consumption rate from glass corrosion and the rate of water flow through the vault, this calculation indicates that at the low recharge rate of 0.1 cm/y, the water consumed from glass hydrolysis is of the same order of magnitude as the rate of water flow. Consequently, within the uncertainty of the numbers used here, there appears to be sufficient water at a recharge rate of 0.1 cm/y to react a considerable fraction of the glass and therefore potentially solubilize the majority of the ⁹⁹Tc inventory. However, the calculation also points out the need to account for water loss due to chemical reactions with the glass and how this water loss affects the flow field in the vault. Fortunately, we are designing the AREST-CT code with this capability.

DISTRIBUTION SHEET

To Distribution	From Administrative Systems Resources (62400)	Page 1 of 1
Project Title/Work Order LLW/D4DC1		Date 11/02/95
		EDT No. 603221
		ECN No. NA

Name	MSIN	Text With All Attach.	Text Only	Attach./ Appendix Only	EDT/ECN Only
B. N. Anderson	H6-06				X
N. R. Brown	K6-51	X			
Y. Chen	K2-40	X			
T. H. De Lorenzo	H0-36	X			
C. R. Eiholzer	H0-36	X			
S. H. Finfrock	H0-38	X			
E. J. Freeman	H0-36	X			
D. Y. Garbrick	H0-36	X			
J. S. Garfield	H5-49	X			
G. W. Gee	K9-33	X			
V. G. Johnson	H6-06	X			
C. T. Kincaid	K9-33	X			
R. Khaleel	H0-36	X			
N. W. Kline (10)	H0-36	X			
D. W. Langford	H8-41	X			
A. H. Lu	H0-36	X			
F. K. Mangan	H8-22	X			
F. M. Mann	H0-36	X			
B. P. McGrail	K2-38	X			
D. E. Mitchell	H5-47	X			
H. J. Morel-Seytoux	K6-77	X			
P. R. Rittmann	H6-30	X			
R. D. Van Houten	H8-44	X			
G. F. Williamson	H5-03	X			
Central Files (Original + 2)	A3-36	X			
EM Files (Burstad 1)	H0-34	X			

Analytic and Computational Research, Inc.
 1931 Stradella Road
 Bel Air, CA 90077
 A. K. Runchal

Daniel B. Stephens & Associates, Inc.
 1845 Terminal Drive, Suite 200
 Richland, WA 99352
 M. G. Piepho