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SALT SITE PERFORMANCE ASSESSMENT ACTIVITIES

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INTRODUCTION

ONWI performance activities involve pre- and post-closure assessments and sensitivity and uncertainty analyses of the repository system and its components at potential salt sites currently under consideration. The geologic repository will consist of multiple natural and engineering barriers that physically separate the radioactive waste from the accessible environment after closure. Analytical and numerical methods are used for long-term assessments of the individual components of multiple barriers as well as the overall system. Performance assessment activities include development, integration, verification, benchmarking, validation, and documentation of the computer codes. The following sections provide two brief examples of these activities.

COMPUTER CODES AND THEIR STATUS

Table 1 is a tentative list of over twenty documented computer codes selected for salt site assessments. However, this list is not intended to preclude use of alternative codes which may be available in the future. The codes listed have been documented and initially verified, but further verification and benchmarking using salt-site related benchmark problems in NUREG/CR-3097\* is in progress. Additional benchmark problems are being developed that specifically pertain to the assessments of the potential salt sites.

Site-specific validation or real-world comparisons of predictions by models with physical measurements will be planned wherever possible. While experimental time is limited compared to the times of interest, successfully predicting the results of in situ experiments carried out over several years can demonstrate confidence that the models, based on physical principles, are sufficiently accurate for long-term predictions. In addition, scale model experiments offer the possibility of scaling time such that a few years of experiment

\* "Benchmark Problem for Repository Siting Models", December 1982, prepared for Division of Waste Management, Office of Nuclear Materials Safety and Safeguards, U.S. Nuclear Regulatory Commission, Washington, DC.

time might be equivalent to hundreds or thousands of years of repository time. For example, in heat transfer, an appropriate experiment might consist of an array of small (1-ft long) resistance heaters with a programmed output where the size, heat output, and array dimensions are determined by use of Fourier's and Poisson's law. Time would be normalized by  $a \times t + L^2$  where  $a$  is the thermal diffusivity,  $t$  is time, and  $L$  is the length of heater sources. Thus, for example, if the experimental heaters and array spacings are made 1/10 the active length of the waste packages and planned repository spacings, respectively, one year of experiment time would simulate 100 years of repository time because of the square power of  $L$ . Opportunities exist for similar scaling for other phenomena.

Specific validations are planned in conjunction with the exploratory shaft activities, such as validation of rock mechanics and thermal codes. In addition, results from near-field permeability studies can be correlated with flow models. Further validation studies, including nuclide transport studies, may be conducted in the Test & Evaluation Facility (TEF) if a salt site is selected for a repository.

Laboratory studies can also be used to assist in site-specific validation using samples collected from the prime salt site area. These studies, well in advance of the TEF, can be used to help validate nuclide transport models using groundwater and stratigraphic samples from the site area. Flow experiments with tracers of iodine, strontium, cesium, americium, and technetium may be conducted. A-priori predictions of sorption and nuclide transport can thus be made and confirmed.

WASTE PACKAGE ANALYSES

ONWI is conducting performance analyses of conceptual spent fuel and reprocessed waste packages in salt<sup>(27)</sup>. The current analyses are limited to conditions expected after emplacement and do not consider human intrusion scenarios that violate the integrity of the salt formation. The results address the question of how long the package will last compared to the NRC regulation<sup>(28)</sup> requiring packages to last 300 to 1,000 years.

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Table 1. Performance Assessment Computer Codes

Code Name	Description	Reference
<u>Waste Package Subsystem Analysis</u>		
ORIGEN-2	Isotopic decay-chain analysis to determine radionuclide buildup during reactor operations, and isotopic composition, thermal and radiation output of waste as functions of time.	ORNL-5621 <sup>(1)</sup>
WAPPA	Corrosion, radiation effects, thermomechanical response of canister, and radionuclide leaching and transport from waste package.	ONWI-452 <sup>(2)</sup>
<u>Geochemical Analysis</u>		
PHREEQE	Coupled solution of thermodynamic equilibrium distribution of chemical species (ion neutral species, ion pairs, and complexes) in aqueous solution; evaluation of mass transfer and solution compositions associated with reactions between solid and fluid phases; for equilibrium conditions.	ONWI-435 <sup>(3)</sup>
EQ3/EQ6	Iterative solution of reaction paths to thermal-dynamic equilibrium distribution of chemical species (ion neutral species, ion pairs, and complexes) in aqueous solution; evaluation of mass transfer and solution compositions associated with reactions between solid and fluid phases; for equilibrium and non-equilibrium conditions.	ONWI-472 <sup>(4)</sup>
<u>Thermal Analysis</u>		
TEMP	Finite line source analytical heat transfer.	Wurm, 1981 <sup>(5)</sup>
DOT	2-D finite-element heat transfer using linear and nonlinear thermal properties and time-dependent heat generation.	ONWI-420 <sup>(6)</sup>
HEATING 6/HEATING 5	2-D and 3-D transient finite-difference heat transfer with temperature-dependent thermal properties and time-dependent heat generation.	NUREG/CR-0200 <sup>(7)</sup>
GEOTHER	3-D finite-difference transient 2-phase water flow and heat flow in porous media.	ONWI-434 <sup>(16)</sup>
FTRANS	2-D finite-element transient water flow and radionuclide transport in saturated porous and fractured media.	ONWI-426 <sup>(17)</sup>
<u>Coupled Ground-Water Flow and Thermal/Mechanical Analysis</u>		
STAFAN	2-D finite-element transient coupled water flow and deformation in fractured media.	ONWI-427 <sup>(18)</sup>
MIGRAIN	Brine migration in salt induced by temperature gradient.	ORNL-5818 <sup>(19)</sup>
<u>Radionuclide Transport Analysis</u>		
LAYFLO	1-D analytical solution of radionuclide transport in multilayered porous media (up to six layers).	ONWI-466 <sup>(20)</sup>
MMT	1-D random-walk solution of radionuclide transport with dispersion in heterogeneous porous media.	ONWI-432 <sup>(21)</sup>
UCB-NE	Series of semi-analytical solutions of varying dimensionality, speciation, phenomenology, and boundary conditions. <u>Radiation Dose Analysis</u>	ONWI-360(1) and <sup>(22)</sup> 360(2)
<u>Radiation Dose Analysis</u>		
OACRIN	Chronic or acute inhalation dose from atmospheric pathways.	ONWI-431 <sup>(23)</sup>
PABLM	Chronic or acute external and ingestion dose from aquatic and terrestrial pathways (including drinking water, ingestion of food, and external exposure from water and ground).	ONWI-446 <sup>(24)</sup>

Table 1. Performance Assessment Computer Codes  
(Continued)

Code Name	Description	Reference
<u>Thermal-Mechanical Analysis</u>		
VISCOT	2-D finite-element transient thermo-elastic and nonlinear thermal visco-plastic and elasto-plastic analysis.	ONWI-437 (8)
SALT-4	2-D viscoelastic transient creep of salt using analytical (thermal) and displacement discontinuity (deformation) formulation.	ONWI-429 (9)
STEALTH	2-D finite-difference thermal-hydraulic analysis with nonlinear material behavior of porous geologic media.	ONWI-256 (10)
<u>Ground-Water Flow Analysis</u>		
NETFLO	3-D steady-state water flow in porous media represented by network of links and nodes.	ONWI-425 (11)
FE3DGW	3-D finite-element transient water flow in saturated porous media, with semiautomatic mesh generation.	PNL-2939 (12)
<u>Coupled Ground-Water Flow, Temperature, Solute and Radionuclide Transport Analysis</u>		
TRIPM	2-D finite-element transient water flow and radionuclide transport in saturated and unsaturated porous media.	ONWI-465 (13)
CFEST	3-D finite-element transient water flow, and temperature, solute and radionuclide transport in saturated porous media.	PNL-4260 (14)
SWENT	3-D finite-difference transient water flow, and energy, solute and radionuclide transport in saturated porous media.	ONWI-457 (15)
<u>Analysis of Future Site Changes</u>		
FFSM	Analysis of synergistic effects of short-duration events and long-term processes, with Monte Carlo selection of uncertain variable values; to determine range of future site characteristics that may result from climatic variations, glaciation, sea level changes, folding, faulting, magmatic events, uplift/subsidence, erosion/deposition, salt diapirism, and natural salt dissolution.	ONWI-436 (25)
<u>Statistical, Sensitivity and Uncertainty Analysis</u>		
GRESS	Calculation of derivatives using as input any code written in FORTRAN involving differential or partial differential equations. Provides for automatic establishment of the adjoint code of the input FORTRAN code.	ORNL/TM-8339 (26)

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The waste package configuration being analyzed is the borehole emplacement concept designated Alternate II in ONWI-438.(29) The spent fuel waste form assumed is disassembled PWR fuel pins (SFPWR) and the assumed commercial high level waste form (CHLW) is borosilicate glass. The SFPWR can is surrounded by a 12 cm overpack of 1025 wrought steel and the CHLW canister by a 15 cm overpack. The borehole is assumed back-filled with about 2 cm of crushed salt (assumed 90% theoretical density after some reconsolidation) around the package and up to the floor level. The waste is assumed 10 years old at emplacement, with the CHLW package initially generating 9.5 kW of heat and the SFPWR package 5.5 kW.

The history of the waste package is being computed using the WAPPA code,(2) which is a subsystem model of the combined effects of transient temperatures, stresses, radiation levels, and chemical boundary conditions at the package surface on the corrosion and failure of the package barriers and on the leaching of the waste form. In the present application of WAPPA, the package failure calculation is essentially a one-dimensional radial geometry integration of overpack corrosion rates at the outside of the overpack wall over the time history of the package until the corrosion allowance is exceeded and it is assumed crushed under lithostatic pressure.

Calculations for the two waste types in the Palo Duro basin, for instance, (Fig. 1)(27) shows the CHLW temperature peaking at one year and 230 C and decaying more rapidly than the SFPWR, which peaks at 130 C and five years. The latter contains a higher proportion of actinides which results in a slower decay of heat generation. The temperature-dependent corrosion rates are higher therefore, for CHLW before the crossover point of 350 years but higher for SFPWR after 350 years. Creeping of the salt is expected to close the borehole around

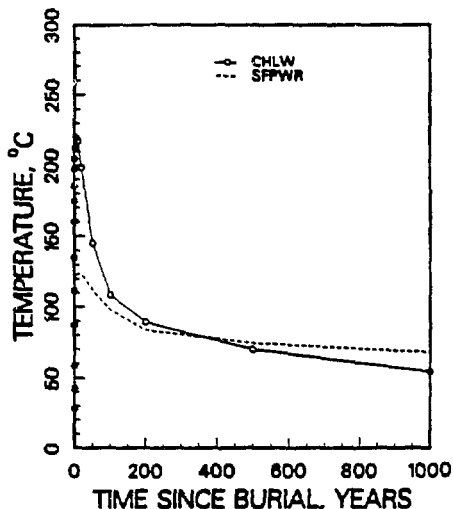


Fig. 1. Temperatures at salt-overpack interface of waste packages in Palo Duro Basin

the waste package during the first few years and maximum stress due to thermal gradients may be exerted on the package during this period, with a gradual decay down to lithostatic pressure during the first decade after burial. Since this occurs so early, it has no significant effect on package life.

Brine flow toward the package is expected to be driven only by the thermal gradient. The brine was allowed to accumulate at the package with no outflow. Transient temperature gradients were computed and input to the brine migration code BRINEMIG [a derivative of code MIGRAIN(30)] to generate the rate of brine inflow to the package. Brine flow theory predicts that brine will not flow below a threshold temperature gradient which is reached in a few hundred years. However, no-threshold brine flow rates were also computed up to 10,000 years. Brine flow was generally greater for CHLW than SFPWR, and was tenfold lower for the Richton dome than the other formations because of the lower water content of its salt. Corrosion rates of 1025 wrought steel are dependent on temperature, brine composition, and radiation level. The corrosion process with high Mg brines (the expected condition for Palo Duro) is anticipated to corrode only 2 cm of the 5 cm corrosion allowance (Fig. 2).(27) Corrosion then stops indefinitely because no more water is available to react with the iron in the overpack. Expected corrosion in a low Mg brine for an SFPWR overpack (in the Richton Dome, for instance) with a 2.5 cm corrosion allowance, predicts package failure only after 7,000 years. This result also applies to low Mg brine intrusion scenarios for all of the salt formations.(27)

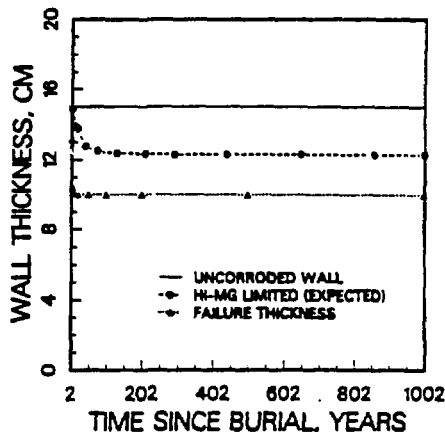


Fig. 2. Effect of brine rate on corrosion of CHLW overpack in Palo Duro Basin

The gross brine accumulations at the package with and without brine flow threshold are shown in Fig. 3 for the SFPWR package in Richton Dome. This figure shows that all of the brine reaching the package is immediately used up by reaction with the overpack. For the CHLW package in the Palo Duro Basin, the greater brine flow may exceed even the high Mg brine corrosion rate during the first 40 years, but at later periods all of it

would be consumed by reaction with the overpack. The net accumulated brine volume is a critical variable in estimating the quantity of radionuclides that will be released from the package under expected conditions in the repository. Even if the package is breached, the product of the solubility limit of the radionuclide in the brine times the net accumulated brine volume is an upper limit on the release of radioactivity from the waste package.(31) It follows that if the net volume of thermally driven brine is nearly zero due to consumption of water by corrosion, the radionuclides released from the package will also be nearly zero.

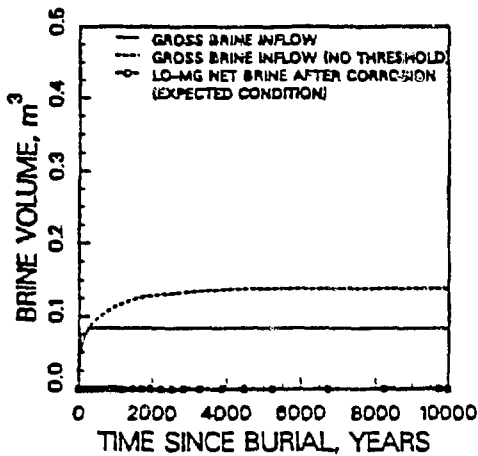


Fig. 3. Accumulated brine at SFPWR waste package in Richton Dome

SITE ANALYSIS

Performance assessments in support of siting activities include ongoing studies of potential sites in domal and bedded salt in Texas, Utah, Mississippi, and Louisiana. Recent site related work has been summarized in a series of papers.(32-34) Results presented for two potential sites in the Palo Duro Basin(34) are summarized here as an example of current work.

Figure 4 illustrates a generalized stratigraphic column of the Palo Duro Basin in the vicinity of the two potential sites. The geologic formations have been divided into three hydrostratigraphic units. The Upper Hydrostratigraphic Unit (HSU A) consists of the Triassic Dockum Group and the Tertiary Ogallala formation. The Dockum and Ogallala are assumed to be hydrologically connected on a regional scale and are grouped into the same hydrostratigraphic unit. Both are fresh water bearing, although the Dockum becomes saline near its base. The Ogallala is heavily used for irrigation, industrial and municipal water supplies throughout the Texas High Plains.

The Middle Hydrostratigraphic Unit (HSU B) consists of Permian age evaporites and shales, including the Lower San Andres Unit 4 salt which is the proposed repository horizon. The Middle Unit is considered a regional aquitard.

The Lower Hydrostratigraphic Unit (HSU C) consists of Pennsylvanian age "granite wash" arkosic sandstone, Pennsylvanian carbonates, and Permian age Wolfcamp carbonates. These deep brine aquifers are separated by various deep basinal shales but may be regionally grouped into one hydrostratigraphic unit.

The Lower Unit brine aquifers have been explored for oil and gas production throughout the Palo Duro Basin. Drill-stem tests provide 5502 formation pressure data points in the basin.(35)

ERA	SYSTEM	SERIES	GROUP	FORMATION	HYDROSTRATIGRAPHIC UNIT (HSU)
CENOZOIC	QUATERNARY	TERTIARY	SANDS	NEOQUATERNARY AND LACUSTRINE DEPOSITS	FRESH-WATER FLOW SYSTEM
				OGALLALA	
				DOCKUM	
MESOZOIC	TRIASSIC	DOCKUM	DOCKUM	TRINITY	HSU A
				DOCKUM	
				DOCKUM	
PERMIAN	PERMIAN	PERMIAN	PERMIAN	TRINITY	SHALE AND EVAPORITE AQUITARD HSU B
				DOCKUM	
				DOCKUM	
				DOCKUM	
				DOCKUM	
				DOCKUM	
				DOCKUM	
				DOCKUM	
				DOCKUM	
				DOCKUM	
				DOCKUM	
				DOCKUM	
PALAEZOIC	PALAEZOIC	PALAEZOIC	PALAEZOIC	TRINITY	DEEP-BASIN FLOW SYSTEM HSU C
				DOCKUM	
				DOCKUM	
				DOCKUM	
				DOCKUM	
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				DOCKUM	

Fig. 4. Generalized hydrostratigraphic column for the Palo Duro Basin area of Texas and New Mexico

Initial examination of the data indicated that the pressures in the deep aquifers were sub-hydrostratic and that equivalent fresh-water heads were several hundred to over a thousand feet below heads measured in the overlying Ogallala. This definite downward potential for flow across the salt section to the deep basin brine aquifers suggests they would be the most likely path for any potential release of radionuclides to the accessible environment.

Potentiometric and permeability data, along with other pertinent geologic data, were used by Intera to develop a regional groundwater model of the Palo Duro Basin. The intent was to define the flow direction and rate in the lower unit, and to determine the sensitivity and uncertainty in the data base.(36) Many simulations were performed using various values for hydraulic parameters combined with varying boundary conditions. Two of these, simulation B and F shown in Fig. 5, are considered representative of actual conditions in the deep basin flow system. The difference between the two simulations is the assumed horizontal conductivity (Kh) of the "granite wash" sandstone along the Amarillo Uplift. If the high

Kh is chosen the uplift acts as a sink and pulls the flow lines to the northeast toward the uplift and then parallel to the uplift as shown in Simulation F. A lower Kh along the uplift, Simulation B, has a less pronounced effect but flow is still to the east-northeast from Deaf Smith and Swisher counties.

Travel times were also calculated for both sites. Table 2 lists the time required for a particle to travel 10 Km when introduced into the Wolfcamp or "granite wash" aquifers at reference positions in Deaf Smith and Swisher Counties.

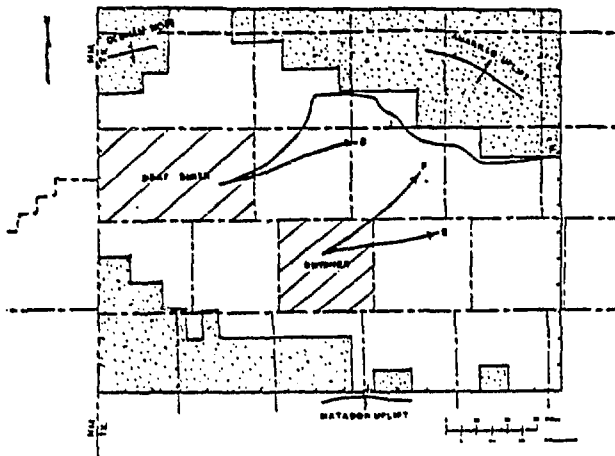


Fig. 5. Particle travel path in Wolfcamp carbonate aquifer (36)

Table 2. 10 Km Particle Travel Times (36)

	DEAF SMITH COUNTY		SWISHER COUNTY	
	TRAVEL TIME yr	TRAVEL TIME yr	TRAVEL TIME yr	TRAVEL TIME yr
Run B (Wolfcamp)	1.1x10 <sup>6</sup>	1.1x10 <sup>6</sup>	1.1x10 <sup>6</sup>	1.1x10 <sup>6</sup>
Run F (Wolfcamp)	8.8x10 <sup>5</sup>	8.8x10 <sup>5</sup>	1.4x10 <sup>6</sup>	1.4x10 <sup>6</sup>
Run B (Granite Wash)	1.5x10 <sup>4</sup>	1.5x10 <sup>4</sup>	1.2x10 <sup>4</sup>	1.2x10 <sup>4</sup>
Run F (Granite Wash)	1.2x10 <sup>4</sup>	1.2x10 <sup>4</sup>	1.4x10 <sup>4</sup>	1.4x10 <sup>4</sup>

Although the travel times are well within DOE and NRC guidelines, there are two important considerations when examining isolation and containment. First, calculations of travel time from the repository to the Wolfcamp using generic values found in literature for permeability and porosity of salt suggest that radionuclides will not escape the repository salt horizon in the first 10,000 years. Using conservative assumptions (10<sup>-3</sup> md) they may travel only about 50 m. There still remains an additional 600 m of evaporites and shales between the repository salt horizon and the top of the Wolfcamp aquifer. These factors

greatly extend travel times under natural conditions, and make the results shown quite conservative. Second, no estimates of retardation are considered in any of the calculations. The assumption is made that radionuclides will travel at the same rate as the groundwater. In reality, retardation will slow down radionuclide migration considerably and will add another margin of safety to the long-term isolation of nuclear waste.

#### SUMMARY

During this year the first selection of the tools (codes) for performance assessments of potential salt sites have been tentatively selected and documented; the emphasis has shifted from code development to applications. During this period prior to detailed characterization of a salt site, the focus is on bounding calculations, sensitivity and uncertainty analysis with the data available. The development and application of improved methods for sensitivity and uncertainty analysis is a focus for the coming years activities and the subject of a following paper in these proceedings. Although the assessments to date are preliminary and based on admittedly scant data, the results indicate that suitable salt sites can be identified and repository subsystems designed which will meet the established criteria for protecting the health and safety of the public.

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