CDM

PROCESSES AND PARAMETERS INVOLVED IN
MODELING RADIONUCLIDE TRANSPORT FROM
BEDDED SALT REPOSITORIES

A TECHNICAL MEMORANDUM

MASTER

For

University of California
Lawrence Livermore Laboratory

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ABSTRACT

CDM/Water Resources Engineers was selected by the Lawrence Livermore Laboratory of the University of California to identify and describe the parameters necessary to model radionuclide transport in salt beds. This technical memorandum is the product of our research.

A proposed plan for disposal of these radioactive wastes generated by nuclear power plants is to store waste canisters in repository sites contained in stable salt formations approximately 600 meters below the ground surface. Among the principal radioactive wastes contained in these canisters will be radioactive isotopes of neptunium, americium, uranium, and plutonium along with many highly radioactive fission products.

A concern with this form of waste disposal is the possibility of groundwater flow occurring in the salt beds and endangering water supplies and the public health. Specifically, the research investigated the processes involved in the movement of radioactive wastes from the repository site by groundwater flow. Since the radioactive waste canisters also generate heat, temperature is an important factor. Among the processes affecting movement of radioactive wastes from a repository site in a salt bed are thermal conduction, groundwater movement, ion exchange, radioactive decay, dissolution and precipitation of salt, dispersion and diffusion, adsorption, and thermomigration. In addition, structural changes in the salt beds as a result of temperature changes are important.

Based upon the half-lives of the radioactive wastes, the period of concern is on the order of a million years. As a result, major geologic phenomena that could affect both the salt bed and groundwater flow in the salt beds was considered. These phenomena include items such as volcanism, faulting, erosion, glaciation and the impact of meteorites.

CDM reviewed all of the critical processes involved in regional groundwater movement of radioactive wastes and identified and described the parameters that must be included to mathematically model their behavior. In addition, CDM briefly reviewed available techniques to measure these parameters.

I.. SUMMARY

This technical memorandum was prepared to develop an annotated list of the parameters necessary to model regional radionuclide transport in groundwater with respect to a bedded salt repository site. In developing the parameter list, we have assumed the boundary conditions and initial values of the variables were known. These items include such things as definition of the depth and areal extent of each stratum, sources and sinks of groundwater and radioactive wastes, geologic occurrences and their geohydrologic effects, and initial groundwater levels and concentrations of radionuclides.

To evaluate regional radionuclide transport, we identified the following eight major processes that should be included in a model:

- Advective Transport
- Diffusion and Dispersion
- Media Deformation
- Sorption
- Dissolution and Precipitation
- Thermal Processes
- Thermomigration
- Radioactive Decay

Based upon these processes, we outlined 26 parameters that must be known and provided a qualitative assessment of how well the parameter values are known. This assessment is summarized in the following table.

PARAMETER SUMMARY

Parameter	Value Certainty
Diffusion coefficient	Needs improvement
Dispersion coefficient*	Uncertain
Specific permeability*	Highly uncertain
Viscosity	Well known
Specific weight	Needs improvement
Porosity*	Uncertain
Specific yield*	Unknown
Dispersivity constant*	Highly uncertain
Rock strength	Well known
Radiation level	Well known
Bulk density	Well known
Void fraction	Needs improvement
Cation exchange capacity*	Uncertain
Selectivity coefficient*	Highly uncertain
Sorption equilibrium constant*	Highly uncertain
Surface area*	Unknown
Spacing of fractures*	Unknown
Solubility	Needs improvement
Dissolution rate	Needs improvement
Specific heat of fluid	Well known
Specific heat of solid/fluid complex	Needs improvement
Density of fluid	Well known
Density of solid/fluid complex	Well known
Thermal conductivity of solid/fluid complex	Needs improvement
Coefficient of thermal dispersion*	Uncertain
Radioactive decay rate	Well known

*Additional research recommended to improve estimates of parameter.

Fifteen of the parameters fall in the categories "well known" and "needs improvement." For present needs in evaluating repository sites this level of certainty should be adequate. Future research efforts should be focused on improving our knowledge of the remaining eleven parameters which fail in the three categories: "uncertain," "highly uncertain" and "unknown." These parameters are denoted in the above table with an asterisk (*).

II. INTRODUCTION

BACKGROUND

One of the major environmental issues facing society today is the safe disposal of radioactive wastes. Since the National Academy of Science's report in 1957, bedded salt deposits have been seriously studied as possible repository sites. Camp Dresser and McKee Inc. has written this technical memorandum for the Lawrence Livermore Laboratory of the University of California to identify and describe the parameters necessary to model radionuclide transport in bedded salt deposits by groundwater. The research focuses on groundwater problems related to the storage of spent fuel generated by nuclear power plants, and specifically, on those processes which might effect regional groundwater resources.

A primary concern of waste disposal in bedded salt deposits is of groundwater intersecting the radioactive waste material and transporting radionuclides to the biosphere. This technical memorandum describes the processes that are important in transporting radioactive wastes from the repository site by groundwater flow. In addition to the earth's natural thermal gradient, radioactive waste canisters will generate heat; consequently, temperature will be an important factor. Among the processes affecting movement of radioactive wastes from a repository site in a bedded salt deposit are thermal convection, groundwater movement, ion exchange, radioactive decay, dissolution and precipitation of salt, dispersion and diffusion, adsorption, and thermomigration. In addition, structural changes in bedded salt deposits as a result of temperature changes may be important.

Due to the long half-lives of the nuclides involved, these wastes must be isolated from the biosphere for periods of time measured in terms of centuries. As a result, major geologic phenomena that could affect groundwater flow in bedded salt deposits must be considered. These phenomena

include items such as volcanism, faulting, erosion, glaciation and the impact of meteorites. Because of the limited time available for this investigation, the affects of catastrophic geological events on the geohydrology of the basin are treated as charged boundary conditions. No attempt has been made to evaluate the causes or likelihood of these events, only their effect on the geohydrology.

This technical memorandum will be incorporated with other research efforts sponsored by Lawrence Livermore Laboratory this year to produce the Task 2 - Fiscal Year 1979 Annual Report. The annual report will describe site suitability criteria for the disposal of high level radioactive wastes at depth. The annual report will be disseminated nationally to provide part of the technical information necessary to make policy decisions about radioactive waste disposal.

SCOPE OF WORK

The scope of work undertaken by Camp Dresser and McKee Inc. under purchase order number 4779209 covers two basic tasks. These tasks are described as follows:

- Task 1 - Develop an annotated list of the parameters necessary to model regional radionuclide transport in groundwater with respect to a bedded salt repository site. The parameter list shall include the parameter definition and a qualitative discussion of the importance of each parameter relative to the models, and a quantitative discussion of the difficulty of predicting the parameter values.
- Task 2 - Review those sections of LBL-7096, "Geotechnical Assessment and Instrumentation Needs for Nuclear Waste Isolation in Crystalline and Argillaceous Rock," that pertain to hydrology. The review shall focus on how well the hydrologic instrumentation needs described in LBL-7096 relate to the hydrologic measurement needed to evaluate a bedded salt deposit as a repository site.

This technical memorandum covers the work conducted under Task 1.

PROJECT ORGANIZATION

Preparation of this technical memorandum was accomplished through the direction and efforts of the project's co-Principal Investigators, Donald E. Evenson and Thomas A. Prickett. Major portions of the memorandum were prepared by Beverly L. Herzog, Patricia A. Showalter, and Michael C. Voorhees. Constance Morris and Becky Wilson provided technical and editorial support in the preparation of the memorandum.

Terry Steinborn and Tom Naymik of the Lawrence Livermore Laboratory provided valuable assistance and guidance in preparing this memorandum. Their helpful reviews of the draft report is appreciated.

III. PROBLEM DESCRIPTION

GEOLOGIC FORMATIONS

In the past few decades light water fission reactors have become a major source of power. Spent fuel rods that remain radioactive for hundreds of thousands of years are produced from nuclear power plants. These wastes must be isolated for hundreds of thousands of years, which is longer than any of mankind's institutions or structures have survived. Repositories must be found for these wastes that will isolate the radioactivity from the biosphere without the need of periodic operation and maintenance activities. Because there are geologic formations that have remained stable for many millions of years, repositories for radioactive wastes deep in geologic formations are being considered as possible disposal sites. Over the long time period that high-level radioactive wastes remain dangerous, manmade containers or canisters cannot be expected to last. The geologic formation itself must provide confinement for the radioactivity.

The major formations that are being considered as repository sites are bedded and domed salt deposits; shale, basalt, granite and other crystalline rocks; and sites above the water table. Each of these rock types have low permeabilities and are found in areally and vertically extensive formations. In this technical memorandum we will focus on bedded salt deposits.

GROUNDWATER

Circulating groundwater provides the most likely connection between a repository site and the biosphere. To evaluate each specific location as a possible repository site, an estimate must be made of the time it would take for groundwater to carry radioactive wastes from the repository site to the surface or to any location where it might contaminate a water supply or endanger the public health. Numerous mathematical computer models have

been developed to predict groundwater flow for water supply studies. These models simulate short periods of time and are based on actual data. The length of hydrologic records does not even approach the length of time that groundwater flow must be predicted for radioactive waste disposal sites. The modeling techniques that have been developed for predicting groundwater flow must be refined and modified to take into account processes that may be significant over hundreds of thousands of years but are negligible over tens of years.

Another major difference between the short term geohydrologic modeling that has been done and the long term modeling that must be done for repository sites is the rate of groundwater flow involved. Most of the modeling of groundwater flow has been done for aquifers--formations that serve as water reservoirs and allow water to flow freely through them. Radioactive waste repositories will be located in aquicludes--formations that contain little water and allow only extremely slow groundwater flow through them. Factors such as dispersion, which are generally insignificant in aquifer modeling, could be very important in long-term aquiclude modeling of point sources of radioactivity.

Our purpose in this technical memorandum is to identify and describe the processes and parameters that must be considered to model regional groundwater migration in bedded salt deposits. Because bedded salt is generally found in a sequence of other rock types, the effect of the other rock types on the radioactive groundwater migration must be considered.

BOUNDARY CONDITIONS

Figure 1 illustrates a typical geohydrologic cross section within which a bedded salt deposit exists. The illustration shows that layering exists in the geologic column with numerous types of deposits of varying permeabilities and that a wide variety of boundary conditions are possible. It is not meant to show detail, specific layering sequences, or possible groundwater flow directions.

FIGURE 1

TYPICAL CROSS SECTION OF HYDROGEOLOGIC ENVIRONMENT

Explanation:

Symbol

Hydrogeologic Characteristics

- A Medium to high permeability deposits - typically sands, gravels, glacial materials.
- B Low to medium permeability deposits - typically salts, clays, and shale.
- C Medium to high permeability deposits - typically sandstones and basalts.
- D Low to high permeability deposits - typically dolomite and limestone.
- E Very low to low to medium permeability - typically combinations of interbedded shales, sandstones and limestones.
- F Very low permeability bedded salt deposits.
- G Low to medium permeability deposits - typically sandstones.
- H Very low to low permeability deposits - typically basement rocks, granites.

In fact, no groundwater flow directions are shown in Figure 1 simply because flow may be driven in any direction depending upon the existence of a potential field. The potential field will be three-dimensional (even though a two-dimensional field is implied in Figure 1). According to a discussion given in Reviews of Modern Physics (1978), the configuration of the potential field depends on at least four factors:

1. The particular forces or potentials that act within the region (e.g., gravity, chemical, or temperature potentials),
2. the geometry of the region within which the potentials exist,
3. the existing boundary conditions, and
4. the nature and variation of properties that control the flow within the region.

When these factors are completely defined, the resulting potential dictates the flow directions and velocities throughout the field.

It is popular to focus attention on the gravity potential wherein the configuration of the water table is the driving force related to groundwater flow. We believe that other potentials (chemical, and particularly the thermal related forces) are just as important, if not more important, to the flow of groundwater at depths dictated by radioactive waste isolation needs.

Figure 1 implies a two-dimensional system. This is not the case. We consider the cross section to be only part of a groundwater basin that is a closed three-dimensional system wherein all waters entering the system also exit within the same system. The side and bottom boundaries are considered impermeable boundaries. Water moves into and out of the system only through the upper water table boundary. (However, this is not to say that thermal sources outside these geohydrologic boundaries do not come into play.)

One must be cautious about choosing groundwater divides as lateral boundaries of the system since these divides are movable either by manmade groundwater pumping processes or by natural long-term climatic and erosional phenomena.

We have addressed the regional aspects of radionuclide transport. In this respect, the geometry and boundary conditions of the repository can be considered as a point source or sink within the bedded salt deposit of the system shown in Figure 1. Emission of heat, rates of radionuclide release to the groundwater, and production or absorption rates related to moisture or gases generated within the repository and transmitted to the neighboring groundwater are assumed to be given parameters (devised possibly by other researchers studying local effects of radionuclide transport).

We have assumed that major boundary conditions and the basin geometry mentioned above are given parameters. In addition, such processes as volcanism, faulting, erosion, and such items as sabotage, nuclear warfare, drilling and the impact of meteorites will not be addressed herein, but will be considered as given mechanisms of nuclide containment failure.

Finally, we have assumed that source and sink functions such as groundwater pumpage, groundwater recharge rates, thermal heat production rates from depths below the repository, or groundwater injection rates are all known.

A typical problem scenario would be definition of the geometry of the groundwater basin, setting of numerous boundary conditions related to radionuclide, chemical, gravity, and thermal considerations, assigning parameter values to the fluid/porous media sequences, and finally, solving the equations of mass transport.

Within these assumptions and limitations we have described the major processes that must be included in a regional model of groundwater transport of radionuclides from a repository in a bedded salt formation. The following chapter describes these processes and defines the input parameters that must be known to adequately model them.

IV. PARAMETER DESCRIPTIONS BY PROCESS

PROCESSES INVOLVED IN REGIONAL WASTE MIGRATION

The purpose of this chapter is to review parameters involved in the significant physical, chemical, thermal and nuclear processes that together determine the pattern of radionuclide contaminant migration in bedded salt deposits. Although the main thrust concerns flow mechanisms in salt deposits, we have not ignored the remaining parameters in the geologic column that are also involved in the total hydrogeologic environment.

We have chosen to discuss parameters as they relate to selected physical, chemical, thermal, and nuclear processes that are likely to be involved in the total contaminant mass transport process. The processes included in the physical category are advective transport, dispersion, and medium deformation. The chemical process group includes diffusion, sorption, dissolution, and precipitation. Thermal related processes include conduction, radiation, and convection and thermomigration effects. The only nuclear process included is radioactive decay.

In assembling the parameter list, the process involved is described and appropriate process equations given for explanatory reasons. It should be mentioned that the process explanations are given to illustrate where the parameters fit into the overall problem of radionuclide transport. There is no explanation as to how all of the process equations fit together.

The parameter list is given in each of the following sections along with tables of parameter values found in the literature search. One must be cautious in using the parameter values since the lists are not exhaustive. The values given are for the purpose of outlining general ranges of values and illustrating their uncertainty.

As a final note, we realize that there are other processes and parameters that may be involved such as electric, magnetic, and osmotic processes in addition to partially saturated flow concepts, steam generation by deep geothermal activity, and multi-liquid flow problems related to possible existence of nearby petroleum and gas. We would have preferred to follow up on these processes and conditions; however, time and budget restraints overruled.

ADVECTIVE TRANSPORT

Process Definition

Advective transport is the process which moves dissolved substances through porous media. The parameters and variables involved in this process are shown below:

<u>Parameters</u>	<u>Process</u>	<u>Variables</u>
specific permeability	Advective Transport	velocity
viscosity		pressure
specific weight		concentration
porosity		
specific yield		

Mathematically, a one-dimensional advective transport process under steady flow conditions* can be expressed as

$$M = QC = vAC \quad \dots \dots \dots (1)$$

* It is not likely that the relative short-term effects of unsteady flow will have to be considered in the large time frame of concern in this report. Therefore, the artesian storage coefficient parameter is neglected.

where

M = rate of advective transport (gm/sec)

Q = flow rate (cm/sec)

C = concentration (gm/cm)

v = apparent velocity (cm/sec)

A = gross cross-sectional area (cm²)

For one-dimensional flow the apparent velocity is computed using Darcy's Law which is expressed as

$$v = k \frac{\gamma}{\mu} \frac{\partial h}{\partial x} \dots \dots \dots (2)$$

where

k = specific permeability (cm²)

γ = specific weight (dynes/cm³)

μ = viscosity (poises)

h = pressure head (cm)

x = distance (cm)

The actual velocity of water particles moving through a porous media varies considerably depending upon the sizes and distribution of the pore spaces in the media and the paths connecting the pore spaces. On the average, we can expect the average actual velocity to be determined by the average pore space involved in the mass transport. The average pore space should be somewhere between the porosity and specific yield of the media. In other words,

$$\frac{v}{S_y} \leq v_a \leq \frac{v}{\eta} \dots \dots \dots (3)$$

where

- v = apparent velocity (cm/sec)
- v_a = actual velocity (cm/sec)
- η = porosity (dimensionless)
- S_y = specific yield (dimensionless)*

Actual velocity, v_a , measures the average distance a water particle will travel per unit time. It is the key variable that must be calculated in the advective transport process. Most investigators use porosity to estimate actual velocities. However, in media with low permeabilities, the difference between porosity and specific yield becomes large and it is important to estimate the average pore space involved in the advective transport process.

Process Parameters

To model the advective transport process, five process parameters must be known; these parameters are:

- specific permeability
- viscosity
- specific gravity
- porosity
- specific yield

The following table presents a summary of the reported values and degree of certainty in estimating values for these parameters. Detailed descriptions of each parameter are described in the following sections.

*Specific yield is also referred to as "effective porosity".

Parameter	Reported Values	Degree of Certainty
specific permeability	10^0-10^{-15} darcys	highly uncertain
viscosity	1.8-0.2 cp	well known
specific density	1.04-0.90 gms/cm ³	needs improvement
porosity	0.5-10%	uncertain
specific yield	none	unknown

Specific Permeability (k)

Todd (1959) describes specific permeability as an intrinsic property of the medium and defined as

$$k = Cd^2 \quad (4)$$

where

k = specific permeability (cm²)

d = representative grain diameter (cm)

C = dimensionless constant

The constant C is determined by properties of the medium other than a representative grain diameter; these properties include porosity, packing, and grain size distribution and shape.

Referring to salt beds, little information was found concerning its specific permeability. Bredenhoeft, et al. (1978), computed a permeability of 0.3×10^{-7} darcys* to restrict transport to 1 km in 10,000 years and reported the value as "not particularly low for natural rock materials." Salt was included as a low permeability media.

Ekren, et al. (1974), reported values of "interstitial permeability of salt of 0.7×10^{-7} to 1.3×10^{-7} gpd/ft². Assuming these represent values at 60 F (the temperature used to define the laboratory or standard coefficient of permeability), the equivalent value of specific permeability can be computed as

$$k = K_s \frac{\mu}{\gamma} = 18.2 K_s \dots \dots \dots (5)$$

where

K_s = laboratory coefficient of permeability (gpd/ft)
(sometimes called hydraulic conductivity)

Using this conversion factor, the range of reported values mentioned above becomes

$$\begin{aligned} \text{max} &= 18.2 (0.7 \times 10^{-7}) = 1.3 \quad \text{darcys} \\ \text{min} &= 18.2 (1.0 \times 10^{-8}) = 2.4 \times 10^{-3} \text{ darcys} \end{aligned}$$

According to Todd (1959), specific permeabilities in this range represent "poor aquifers" and are typical of such media, as very fine sands, silts, mixtures of sand, silt and clay, glacial tills, stratified clays, etc.

* 1 darcy = 3.987×10^{-8} cm²

Dames and Moore (1978), in a report for the Office of Waste Isolation, presented permeability estimates for rock salt (halite), bedded salts from the Saline and Permian Basins, and typical rock-mass formations of salt. The reported values, as well as their equivalent "specific permeability" values (assuming measurements were made at 20 C), are presented in the following table:

Salt Media	Reported Permeability	Specific Permeability
Intact Salt (Halite)	1.7×10^{-15} to 1.0×10^{-2} ft/yr	0.62×10^{-15} to 0.36×10^{-2} darcys
Salina Basin	1.0×10^{-18} ft/min	0.19×10^{-14} darcys
Permian Basin	1.0×10^{-19} ft/min	0.18×10^{-14} darcys
Salt Rock Mass	1.7×10^{-15} to 1.1×10^{-2} ft/yr	0.62×10^{-15} to 0.40×10^{-2} darcys

The values reported by Dames and Moore (1978) are representative of media that range from poor aquifers to impervious material.

Permeabilities of other geologic formations are also important. The above discussion is primarily aimed at permeabilities of various types of salt. Although consideration of flow through salt is important, flow through any part of the geohydrologic system of Figure 1 should be considered. In this respect, the table below gives values of hydraulic conductivity, K_s (from equation 5, $K_s = \frac{k \gamma}{\mu}$) for various hydrogeologic formations. The table below was taken from Reviews of Modern Physics (1978).

HYDRAULIC CONDUCTIVITIES OF GEOLOGIC MEDIA

Material	Hydraulic Conductivity (cm/sec)
Slate	1.1×10^{-9}
Quartzite	1.6×10^{-9}
Graywacke	2.6×10^{-9}
Clay, montmorillonite	4.7×10^{-9}
Till, clay-loam (intergranular)	$2.7-6.0 \times 10^{-9}$
Salt, bedded ^a	6.3×10^{-9}
Till, clay-loam (fractured)	1.8×10^{-7}
Shale ^b	$0.7-2.0 \times 10^{-7}$
Siltstone	1.2×10^{-7}
Limestone, argillaceous	0.9×10^{-7}
Dolomite	0.9×10^{-6}
Sandstone, silty	2.2×10^{-6}
Limestone	6.6×10^{-6}
Silt	$1.0-7.2 \times 10^{-5}$
Graywacke (fractured)	3.9×10^{-5}
Sandstone, coarse	0.9×10^{-3}
Sand, river alluvial	1.7×10^{-2}

^a Measurements for some salts give values as high as 1.5×10^{-4}

^b Measurements for some shales give values as low as 0.8×10^{-10}

Strictly speaking, the above table should have corresponding temperatures along with the hydraulic conductivity as the two parameters are related through Equation 5. In any case, order of magnitudes in the above table are valid.

A substance is considered anisotropic if its properties are directional. Permeability is the most common parameter to be anisotropic. This is the case in most stratified material where the flow proceeds more easily along the planes of deposition than across them. It is sufficient to be aware that this process takes place and that indeed, permeability values quite frequently can not be considered equal in all three principal directions.

Viscosity (μ)

Lee and Sears (1955) define viscosity of a fluid as "the ratio of shearing stress to rate of change of shearing strain." Basically, it is a measure of the friction force that must be exerted to cause one layer of a fluid to slide past an adjacent layer of fluid. It can be expressed as

$$\mu = T / \frac{dv}{dx} \dots\dots\dots (6)$$

where

- μ = absolute viscosity (dyne-sec/cm²)
- T = shear stress per unit area (dynes/cm²)
- $\frac{dv}{dx}$ = maximum velocity gradient (sec⁻¹)

The intensity of the viscous shear is important in determining internal energy loss in fluid motion. Viscosity is highly dependent on temperature and for fluids it decreases with increasing temperature. In other words, the higher the temperature, the easier it is for adjacent fluid layers to move relative to one another. Values for the viscosity of water have been well established. According to the 39th Edition of the Handbook of Chemistry and Physics (1957-58), the viscosity of water varies with temperature according to the following table:

Temperature (°C)	Water Viscosity (cp)	Temperature (°C)	Water Viscosity (cp)
0	1.792	90	0.316
10	1.308	100	0.284
20	1.005	110	0.256
30	0.801	120	0.232
40	0.656	130	0.212
50	0.549	140	0.196
60	0.469	150	0.184
70	0.412	160	0.174
80	0.356		

Note: 1 centipose (cp) = 10^{-2} poise;
 1 poise = 1 dyne sec/cm²

Specific Weight (γ)

The specific weight of water is the force or weight per unit volume and is defined as:

$$\gamma = \rho g \quad \dots \dots \dots (7)$$

where

γ = specific weight (dynes/cm³)

ρ = density (gm/cm³)

g = gravity (980 cm/sec²)

The relative density of pure water varies with temperature and according to the 39th Edition of the Handbook of Chemistry and Physics (1957-58), the values at atmospheric pressure are as shown in the following table:

Temperature (°C)	Relative Density of Water (gm/cm ³)	Temperature (°C)	Relative Density of Water (gm/cm ³)
0	0.99987	90	0.96534
10	0.99973	100	0.95838
20	0.99823	110	0.9510
30	0.99567	120	0.9434
40	0.99224	130	0.9352
50	0.98807	140	0.9264
60	0.98324	150	0.9173
70	0.97781	160	0.9075
80	0.97183	170	0.8973

Relative density is the absolute density of pure water relative to the density of water at 4°C. At this temperature, pure water is at its maximum density (0.999973 gm/cm³) and has a relative density of 1.0 gm/cm³. Since the two values are virtually identical, absolute and relative densities can be used interchangeably.

For water flowing in bedded salt, density will also change with pressure and salinity. Water is an elastic fluid and according to Camp (1963), "has a modulus of elasticity of about 300,000 psi; which indicates a volumetric decrease of about 0.000048 for each atmosphere of pressure." (Note: one atmosphere of pressure = 1.0132×10^6 dynes/cm or 33.90 feet of water.) Assuming a potential pressure range of 100 atmospheres, the maximum pressure effect would be a volumetric decrease of 0.0048 which is not particularly significant. As a result, the effect of pressure on density can be ignored.

Salinity effects on density are far more important. La Fond (1951) presents a procedure to compute the density of sea water based on values of temperature, salinity or chlorinity and pressure. However, even though

salt (NaCl) is the predominant mineral in sea water, the temperature and pressure ranges to be expected in salt beds near repository sites will be greater than the ranges included in the data used by La Fond (1951). As a result, density-temperature-salinity (and perhaps pressure) relationships are needed. Based on our brief literature review, we did not find them. However, for modeling purposes, it may be sufficient to use relationships developed simply from chemical mass balances which can be computed.

Porosity/Specific Yield

Porosity is defined as the percentage of total void space to the total volume of the mass. Specific yield, on the other hand, represents the volume of water that will drain by gravity from the void space relative to the total volume of the mass. The remaining water is held in the voids by molecular and surface tension forces and is described by the specific retention of the media.

Dames and Moore (1978) and Ekren (1974) have reported porosity values for salt beds. These values ranged from less than 0.3 percent to 10 percent and are summarized in the following table. Porosity values are substantially less than those encountered in aquifers, presumably as a result of the crystalline structure of the salt.

Source	Salt Bed Porosity
Dames and Moore (1978)	
Intact Salt (Halite)	1.4-10%
Salina Basin Salt	< 0.5%
Permian Basin Salt	
New Mexico	< 3.0%
Kansas	< 0.5%
Salt Rock Mass	0.5%
Ekren (1974)	< 1.0%

During our brief literature search we were not able to uncover any values for specific yield of salt beds. However, Dames and Moore (1978) did report values for moisture content in the range of 0.03 to 0.75 percent with all values except for one less than 0.25 percent. If these values are considered as the minimum possible levels of specific retention, the potential range for specific yield is 0.24 to 9.97 percent or between 50 - 100 percent of the porosity.

Walton (1970) reports on the specific yield of other geologic formations as given in the table below.

Rocks	Specific Yield (Percent)
Clay	1-10
Sand	10-30
Gravel	15-30
Sand and gravel	15-25
Sandstone	5-15
Shale	0.5-5
Limestone	0.5-5

DIFFUSION AND DISPERSION

Process Definition

Diffusion and dispersion are two processes that tend to disperse or distribute dissolved constituents within a porous media. Both processes are irreversible and occur under both steady and unsteady flow conditions. The parameters and variables involved in these processes are shown below.

<u>Parameters</u>	<u>Processes</u>	<u>Variable</u>
diffusion coefficient dispersion coefficient	Diffusion and Dispersion	concentration

Mathematically, the mass transfer of a dissolved substance by both diffusion and dispersion are represented as the product of a coefficient times the local concentration gradient.

For one-dimensional flow in an isotropic media, these processes can be described as

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial C}{\partial x} \right) \dots \dots \dots (8)$$

where

C = concentration (mg/l)

D = D_m + D_I

D_m = molecular diffusion coefficient (cm²/sec)

D_I = longitudinal dispersion coefficient (cm²/sec)

t = time (seconds)

x = distance (cm)

In most cases the molecular diffusion coefficient is small compared to the dispersion coefficient.

In the case of two-dimensional flow with negligible molecular diffusion, the dissolved material can disperse both in the direction of flow and transverse to it. Borg, et al. (1976) described the two dimensional process as

$$\frac{\partial}{\partial x} \left[D_{xx} \frac{\partial C}{\partial x} + D_{xy} \frac{\partial C}{\partial y} \right] + \frac{\partial}{\partial y} \left[D_{yy} \frac{\partial C}{\partial y} + D_{yx} \frac{\partial C}{\partial x} \right] \dots \dots (9)$$

where

$$D_{xx} = D_I \frac{v_x^2}{v^2} + D_{II} \frac{v_y^2}{v^2}$$

$$D_{yy} = D_I \frac{v_y^2}{v^2} + D_{II} \frac{v_x^2}{v^2}$$

$$D_{xy} = D_{yx} = (D_I - D_{II}) \frac{v_x v_y}{v^2}$$

and

- D_I = longitudinal dispersion coefficient (cm²/sec)
- D_{II} = transverse dispersion coefficient (cm²/sec)
- v_x = velocity in x-direction (cm/sec)
- v_y = velocity in y-direction (cm/sec)
- v = magnitude of velocity vector (cm/sec)

For the special case of the velocity vector in the x-direction, Equation (9) simplifies to:

$$\frac{\partial}{\partial x} (D_I \frac{\partial C}{\partial x}) + \frac{\partial}{\partial y} (D_{II} \frac{\partial C}{\partial y}) \dots \dots \dots (10)$$

These relationships apply to the special conditions of an isotropic media. In other words, a media whose longitudinal and transverse dispersion coefficients are the same regardless of the direction of flow.

For modeling purposes, both diffusion and dispersion coefficients need to be estimated. The following paragraphs describe procedures that have been reported in the literature for estimating values for these parameters.

Diffusion Coefficients

Molecular diffusion represents the mixing that takes place as a result of the movement of both ions and molecules in a liquid. Compared to typical values of advective transport and dispersion, molecular diffusion is usually very small and generally ignored. However, Rumer (1972) found that when the Reynolds Number is less than 0.001, molecular diffusion becomes important. Reynolds Numbers in this range occur when seepage velocities are very low and the median diameter (d_{50}) of the media is very small.

Values for molecular diffusion coefficients depend upon the solute, solute concentration, and temperature. For salt (NaCl) dissolved in pure water, Camp (1963) reported the following diffusion coefficients as a function of temperature:

Temperature (°C)	Molecular Diffusion Coefficient (cm/sec)
5	0.88×10^{-5}
10	1.03×10^{-5}
15	1.18×10^{-5}
20	1.38×10^{-5}
25	1.62×10^{-5}
30	1.85×10^{-5}

concentration = 0.05 molal

As mentioned earlier, for most practical cases molecular diffusion can be ignored because it is usually small relative to dispersion. However, in those cases where dispersion is in the same order of magnitude as diffusion, it may become important to include the effects of molecular diffusion

when dealing with radionuclides with exceptionally large half-lives (greater than 10,000 years).

Within the brief period allowed for this literature search, we did not uncover any values for molecular diffusion coefficients for dissolved radionuclides. Additional reviews of the literature should be undertaken if future research efforts point out conditions where molecular diffusion can be significant.

Dispersion Coefficients

Dispersion in porous media takes place because of the complex geometry of the pore spaces and the vast number of possible flow paths through the pore spaces. As a fluid moves through a porous medium, those particles that travel through the large pore spaces and along the least resistant paths will move faster than the other particles. These differences in interstitial velocities induce longitudinal mixing or dispersion. As a result of the complexity of the flow paths, some particles will also move laterally and transverse dispersion results. Hence, dispersion takes place in the direction of flow as well as transverse to it.

Longitudinal Dispersion

Several investigators have reported different but similar relationships for estimating longitudinal dispersion coefficients. For example, Scheidegger (1961) indicated that the longitudinal dispersion coefficient could be estimated as a simple function of the seepage velocity times a "dispersivity" constant as follows:

$$D_L = dv_s \dots \dots \dots (11)$$

where

d = dispersivity (cm)

v_s = seepage velocity (cm/sec)

He indicated the dispersivity value was a property of the porous media and dependent upon the geometry of the pore structure.

In 1962, Rumer reported the results of some dispersion experiments using quartz gravels and glass beads as media. He found that the longitudinal dispersion coefficient was related to the seepage velocity by the following relationship:

$$D_I = \alpha v_s^m \quad \dots \dots \dots (12)$$

where

α = constant

m = exponent

His results and media data were:

Media	d_{50} (cm)	d_{60}/d_{10}	α	m
Quartz gravel	0.165	1.26	0.20	1.083
Glass beads	0.039	1.13	0.027	1.105

About the same time, Banks and Jerasate (1962) were conducting dispersion experiments with a gravel of near uniform size ($d_{50} = 0.546$ cm). They found they could approximate the value of the longitudinal dispersion coefficient with the expression

$$D_I = A_0 d_{50} v_s \dots \dots \dots (13)$$

where

$A_0 = \text{constant} = 1.92$

$d_{50} = \text{median grain diameter (cm)}$

$v_s = \text{seepage velocity (cm/sec)}$

They found the relationship to be generally valid for a range in Reynolds Numbers from 17 to 164.

Harleman, et al. (1963) summarized some earlier research by Ebach and White (1958) who found the following relationship:

$$\frac{D_I}{v} = \alpha_0 \left[\frac{d_{50} v_s}{v} \right]^n = \alpha_0 R^n \dots \dots \dots (14)$$

where

$\alpha_0 = 1.92$

$n = 1.06$

$R = \text{Reynolds Number}$

$v = \text{kinematic viscosity (stokes)}$

Several years later, Harleman, et al. (1963) confirmed the relationship with some experiments using seven types and sizes of spheres and three different types of sands. The results of their experiments were:

Media	d_{50} (cm)	d_{60}/d_{10}	α_v	n
Spheres	0.039-0.20	1.00-1.15	0.66	1.2
Sands	0.045-0.14	1.08-1.15	0.90	1.2

More importantly, Harleman, et al. (1963) observed the relationship between the dispersion coefficient and specific permeability. Remembering that the specific permeability is dependent upon the media grain size according to the relationship

$$k = C d_{50}^2 \dots \dots \dots (15)$$

where

k = specific permeability (cm^2)
 C = constant of the media

For the media used in their experiments, they found an average value for C to be

$$C = 6.15 \times 10^{-4}$$

Rearranging Equation (15)

$$d_{50} = \sqrt{\frac{k}{C}} \dots \dots \dots (16)$$

and substituting this equation into Equation (14) results in the following expression

$$\frac{D_I}{v} = \alpha_n \left[\sqrt{\frac{k}{c}} \frac{v_s}{v} \right]^n \dots \dots \dots (17)$$

This expression allows the longitudinal dispersion coefficient to be estimated from the value of the specific permeability.

They also observed that their preliminary evidence indicated the value of n for uniform or nearly uniform media was 1.2 and it approaches unity for highly nonuniform media.

Lateral Dispersion

Li and Lai (1963) described lateral dispersion experiments using ten different media. They started out to test the hypothesis that the lateral dispersion coefficient could be determined from the relationship

$$D_{II} = \frac{3}{16} d_{s0} v_s \dots \dots \dots (18)$$

Using a variety of media including spheres, sand, pebbles and gravel, they found

$$\frac{D_{II}}{v} = \beta \left[\frac{v_s d_{s0}}{v} \right]^{3/4} \quad 0.3 < R < 10 \dots \dots \dots (19)$$

and

$$D_{II} = \gamma \left[\frac{v_s d_{s0}}{v} \right]^{4/3} \quad 10 < R < 380 \dots \dots \dots (20)$$

where

D_{II} = lateral dispersion coefficient
 β, γ = constants

Values reported for β and γ were

Media	β	γ
Spheres	0.03	-
Sand	0.08	-
Pebbles	0.12	0.03
Gravel	-	0.02

Another method used to estimate the lateral dispersion coefficients is by the ratio of longitudinal to lateral dispersion coefficients. Among the values reported in the literature are:

D_I/D_{II}	Reference
7.0 to 22.7	Bear (1961 b)
24 (max)	Blackwell (1959)
3.3	Konikow and Bredehoeft (1974)

Comparing the results of Harleman, et al. (1963) with Li and Lai (1966) for both sand and spheres, we found the following:

Media	Reynolds Number	D_I/D_{II}
Sand	0.1	3.4
Sand	1.0	11.2
Spheres	0.1	6.4
Spheres	1.0	17.5

In this comparison, the ratio of longitudinal to lateral dispersion coefficients ranged from 2.4 to 17.5 depending upon the Reynolds Number and the media. Use of the ratio D_L/D_{LL} appears to be an over-simplification unless the coefficients for Equation (19) are simply not known or not available.

Anisotropic Conditions

Both Schiedegger (1961) and Bear (1961 a) addressed the problems associated with dispersion in an anisotropic porous media. Their research was theoretical and pointed out the complexities in dealing with an anisotropic media. Instead of the two dispersion coefficients needed in isotropic media, the dispersivity becomes a fourth rank tensor and 36 independent components need to be estimated. This level of complexity has precluded dealing with anisotropic dispersion in practical modeling efforts.

Calibrated Dispersivity Values

In calibrating groundwater transport models, the dispersivity values are often the parameters that are adjusted to obtain calculated solute concentrations that agree with measured values. In theory, dispersivity values should correspond to those measured in the laboratory. However, there are macro-scale effects that are included in models and these effects tend to increase the apparent dispersivity. These effects include local changes in stratigraphy, solute stratification, sampling errors, anisotropy and approximations in the model.

Borg, et al. (1976) and Anderson (1979) have summarized dispersivity values obtained by calibrating groundwater transport models. These values are presented in the following table. For longitudinal dispersivity, the values ranged from 11.6 to 91 m. and are considerably greater than values observed in the laboratory. Several researchers have found that laboratory values of dispersivity to be roughly 0.5 to 2 times the median grain diameter. These factors suggest dispersivity values of less than 1 cm. and more typically less than 0.1 cm.

DISPERSIVITY VALUES OBTAINED BY CALIBRATION OF
TRANSPORT MODELS AGAINST OBSERVED GROUNDWATER SOLUTE TRANSPORT
AFTER ANDERSON (1978) AND BORG, ET AL. (1976)

Aquifer and Location	Longitudinal Dispersivity, α_L (m)	Transverse Dispersivity, α_T (m)	Effective Porosity of Aquifer (%)	Reference Source
Cook Mountain Limestone, Tatum Dome, Mississippi	11.6		23	Anderson (1978)
Ocala Limestone, Brunswick, Georgia	61	20	35	Anderson (1978)
Pleistocene glacial outwash sand and gravel, Long Island, New York	21.3	4.3	35	Anderson (1978)
San Andres Limestone, Roswell Basin, New Mexico	21.3		1 to 10	Anderson (1978)
Culebra dolomite member of Rustler Formation, near Carlsbad, New Mexico	38.1		12	Anderson (1978)
Basalt lava flows and inter- bedded sediments of the Snake River Plain aquifer, near Idaho Falls, Idaho	91	137	10	Anderson (1978)
Bonanza King Formation (Lower Carbonate Aquifer) near Nevada Test Site	15		At least 1.5 (see text)	Anderson (1978)
Alluvial aquifer Rocky Mountain Arsenal, Colorado	30.5	30.5	30	Borg, et al. (1976)
Alluvial aquifer, Colorado	30.5	9.2	20	Borg, et al. (1976)

The ratio of calibrated to typical laboratory dispersivity values is in the order of 100 to 1,000. These high ratios indicate that the macro-scale effects dominate the dispersion process in regional groundwater transport models and should receive more attention in further studies.

Summary

For two-dimensional flow, longitudinal and lateral dispersion coefficients can be calculated by the expressions

$$\frac{D_I}{v} = \alpha_0 \left[\frac{d_{50} v_s}{v} \right]^{n_I} \dots \dots \dots (21)$$

$$\frac{D_{II}}{v} = \beta_0 \left[\frac{d_{50} v_s}{v} \right]^{n_{II}} \dots \dots \dots (22)$$

where the coefficients α_0 , β_0 , n_I , n_{II} are dependent upon the porous media. Most experiments have been conducted with relatively porous, permeable media with grain sizes greater than 0.01 cm. These types of media are not typical of expected conditions in bedded salts or sedimentary basins. Hence, additional literature reviews should be conducted to determine if values for these parameters are available.

In model calibration studies, dispersivity values range from 100 to 1,000 times greater than those found in the laboratory. This finding suggests that macro-scale effects related to non-homogeneity are much more important than the dispersion that takes place within small, homogeneous sections of the aquifer. Additional research is needed to better understand these larger scale processes.

MEDIA DEFORMATION PROCESS

The only media deformation processes in salt deposits that are suspected of having a possible effect on regional geohydrology are faulting and fracturing. The "creeping" of the salt that will occur at the repository site will have a very localized effect and is not expected to have a significant effect on regional waste migration.

Process Definition

Fracturing is the process by which rock is broken, generally along a plane. The break in the rock serves as a potential channel for groundwater flow. A fault is a fracture along which movement has taken place. The parameters and variables important with respect to the geohydrology of salt beds are discussed below.

<u>Parameters</u>	<u>Processes</u>	<u>Variables</u>
rock strength	Deformation by:	temperature
radiation level	Fracturing	pressure
	Faulting	radiation level

Unlike the other processes discussed in this section, media deformation is not expected to have an effect on the geohydrologic regime of a bedded salt repository unless certain catastrophic events take place such as meteor impact, volcanicism, or major faulting activity. The likelihood of such events has been quantified by H. C. Claiborne and J. Gera (1974). The following table summarizes their results.

<u>Event</u>	<u>Probability occurrence/year</u>
Catastrophic Meteorite Impact	1.6×10^{-13}
Faulting Through Repository	4.0×10^{-11}
Volcanism Through Repository	too small to be quantified

Since radiation and heat are known to alter the strength of many substances, it was suspected that they might weaken the salt in the repository making it more vulnerable to fracturing and circulating groundwater. As described below, however, the effects of the heat and radiation of the waste canisters will not be sufficient to change the regional geohydrology.

When salt is heated to very high temperatures, it shatters. Bradshaw, et al. (1968) suggested that the rise in pressure caused by heated brine inclusions is the major cause of shattering. The following table, taken from Bradshaw, et al. (1968) lists the fracturing temperature of various salt samples. The canisters themselves are not expected to reach these temperatures, much less the salt surrounding them.

THERMAL STABILITY OF SALT FROM VARIOUS LOCATIONS
FROM BRADSHAW, et al

Location of Sample	Number of Samples Tested	Fracturing Temperature (C°)	Salt Type
Hutchinson, Kansas	30	260-320	Bedded
Lyons, Kansas	8	285-320	Bedded
Fairport Harbor, Ohio	2	380	Bedded
Retsof, New York	2	*	Bedded
Detroit, Michigan	2	290	Bedded
Cheshire, England	1	250	Bedded
Alsace, France			
NaCl	2	240-280	Bedded
KCl	1	*	Bedded
Winnfield, Louisiana	2	*	Dome
Grand Saline, Texas	2	*	Dome
Weeks Island, Louisiana	2	*	Dome

*Indicates that the salt did not fracture up to 400°C

Radiation has a minimal effect on the strength of salt. The following table from Bradshaw, et al. (1968) lists the mechanical properties at 20 C° and 200°C for increasing increments of radiation dosage. The compressive strength of the irradiated salt is less than the unirradiated salt. The radiation seems to have a more severe effect on dome salt than on bedded salt. The decrease in compressive strength indicates that the irradiated salt is more brittle than the unirradiated salt and therefore more subject to fracture. Katrine Holdoway (1974) noted that the additional brittleness of irradiated salt was particularly evident in thin section preparation. However, dosages of 5×10^8 rads are only expected to accumulate within one foot of the waste canister (Bradshaw, et al., 1968).

Decreases in the primary permeability of salt due to increases of pressure have been measured (Lai, 1971 and Reynolds and Gloyne, 1960). The primary permeabilities of salt are so low, that reducing them still further should have no effect on the regional geohydrology.

Shale layers interbedded in the salt have been observed to serve as parting faces in salt mines where creep has occurred (McClain and Bradshaw, 1970). Slippage may occur along these parting faces. The partings also serve as potential groundwater channels. Any partings near the mined area of the repository should heal themselves, because brine will be cooled as it moves away from the heat source thus becoming supersaturated. Salts from the supersaturated liquid will precipitate onto the parting faces plugging the channels. In the case of major faulting and erosion where overburden pressures are significantly reduced, gaps that develop along shale layers could serve as channels for circulating groundwater that might eventually destroy the salt bed. This event is several orders of magnitude less likely than a major fault intercepting the repository as shown in the above table.

PHYSICAL PROPERTIES OF ROCK SALT FROM
HUTCHINSON, KANSAS, AND GRAND SALINE, TEXAS
FROM BRADSHAW ET AL 1968

Type of Salt	Exposure Dose (R)	Comprehensive Strength (psi)	Yield Strength (psi)	Apparent Elastic Limit (psi)	Modulus of Elasticity (psi) x 10 ⁶
<i>At 20°C</i>					
Bedded parallel	0	4200 ± 500	2500 ± 300	1900 ± 300	0.35 ± .06
	10 ⁵	4500 ± 500	2500 ± 150	1900 ± 200	0.32 ± .06
	10 ⁷	4600 ± 400	2700 ± 250	2100 ± 200	0.35 ± .02
	10 ⁸	4600 ± 150	3400 ± 250	2800 ± 200	0.36 ± .09
	5 x 10 ⁸	3500 ± 50	2700 ± 200	2000 ± 300	0.39 ± .07
Bedded perpendicular	0	4000 ± 400	2300 ± 300	1700 ± 200	0.36 ± .17
	10 ⁵	3800 ± 500	1800 ± 250	1400 ± 250	0.35 ± .10
	10 ⁷	4100 ± 400	2300 ± 500	1800 ± 500	0.38 ± .14
	10 ⁸	4000 ± 400	2400 ± 500	1900 ± 300	0.38 ± .06
	5 x 10 ⁸	3500 ± 400	2400 ± 300	1900 ± 250	0.37 ± .11
Dome	0	5600 ± 100	2900 ± 150	2000 ± 100	0.50 ± .05
	10 ⁵	5300 ± 100	2900 ± 150	2000 ± 300	0.51 ± .12
	10 ⁷	5100 ± 200	3000 ± 100	2100 ± 300	0.62 ± .06
	10 ⁸	4100 ± 200	2700 ± 100	1800 ± 200	0.43 ± .04
	5 x 10 ⁸	3600 ± 500	2600 ± 200	1900 ± 50	0.59 ± .12
<i>At 200°C</i>					
Bedded parallel	0	3900 ± 200	1600 ± 200	1400 ± 100	0.09 ± .01
	5 x 10 ⁸	3400 ± 400	1900 ± 250	1800 ± 250	0.12 ± .02
Bedded perpendicular*	0	3600 ± 100	1600 ± 100	1500 ± 150	0.11 ± .01
	5 x 10 ⁸	3300 ± 400	2100 ± 150	1800 ± 100	0.12 ± .02
Dome	0	3600 ± 500	1900 ± 150	1600 ± 200	0.14 ± .01
	5 x 10 ⁸	3100 ± 300	2300 ± 150	1800 ± 200	0.16 ± .01

Bedded parallel: bedded salt, force applied parallel to the planes of stratification
Bedded perpendicular: bedded salt, force applied perpendicular to the planes of stratification

*Only two samples tested

As shown in the event probability table, the chances of catastrophic events deforming the saltbeds and therefore changing their geohydrologic nature is very small. Even if the salt beds were severely fractured by tectonism, volcanism or meteorite impact, salt has healing properties which would reduce their impact. The very existence of ancient saltbeds is evidence of their ability to repel the circulation of groundwater. As Claiborne and Gera (1974) state:

It is generally accepted that faulting of thick salt formations does not lead to the formation of permeable zones; on the contrary, the plastic deformation of salt is known to heal any fracture opening. As a matter of fact, most of the known faults in salt formations confirm the self-healing behavior of halite. Fault breccias, which are common in brittle rocks, are completely unknown in salt formations.

SORPTION PROCESSES

Process Definition

Sorption includes the attenuation processes that cause the flowrate of radionuclides through an aquifer to be much slower than the flowrate of the water itself. "Adsorption, ion exchange, colloid filtration, reversible precipitation and irreversible mineralization" (Burkholder, 1976 and Burkholder, et al., 1976) are all considered sorption. These processes all reduce the velocity with which the dissolved ions travel through the deposit. Instead of flowing straight through the medium at the same rate as the water, the ions are continually going into and out of solution combining with the media and then redissolving into the water. With respect to the migration of radionuclides through bedded salt deposits, adsorption and cation exchange are of particular concern. These sorption processes are considered together because in groundwater modeling their effect has been (Burkholder, 1976) quantified by a single dimensionless coefficient called the sorption equilibrium constant (K) which is calculated from the distribution coefficient or the selectivity coefficient (K_d).

To include the effects of sorption in the advective transport equation (Eqn. 1), the velocity term should be changed to reflect the velocity of the ions instead of the apparent water velocity. The rate of advective transport or the rate at which the dissolved ions travel through the aquifer depends on the velocity of the ions which may be much less than the velocity of the water. The velocity of the ion is related to the velocity of the water by the following equation:

$$v_i = \frac{v_w}{K} \quad (23)$$

where

v_i = velocity of ion (cm/sec)

v_w = velocity of water (cm/sec)

K = sorption equilibrium, constant or retardation coefficient

The sorption equilibrium constant (K) is calculated using the following formula.

$$K = 1 + K_d \left(\frac{1 - \phi}{\phi} \right) \rho \quad (24)$$

where

K_d = selectivity coefficient (ml/g)

ρ = bulk density of medium (gm/cm³)

ϕ = porosity of medium

Sorption encompasses a set of extremely complicated physiochemical processes which are based on many variables. The result of the sorption processes in radionuclide transport is to reduce the velocity at which the radionuclides travel relative to the water velocity. The combined effects of many of the variables with one another are not fully understood and they

are far beyond the scope of this study. For instance, how will the competition between various radionuclides in the groundwater effect the amount of material that is actually sorbed to any particular medium? The parameters and variables that were found to be significant through our literature search are listed below.

<u>Parameters</u>	<u>Processes</u>	<u>Variables</u>
bulk density	Adsorption	ion velocity
selectivity coefficient or distribution coefficient	Ion exchange	ion concentration
porosity		water velocity

Unless otherwise stated, the remaining discussion of sorption phenomena are based on Borg, et al. (1976).

Selectivity Coefficient

The selectivity coefficient or distribution coefficient, K_d , indicates the tendency of a particular solid to combine with a particular ion. For particulate solids such as sandstone or shale, Borg et al. (1976) expressed the selectivity coefficient for an ion A as

$$K_d = \frac{(\text{amount of A in solid phase})/(\text{weight of solid})}{(\text{amount of A in liquid phase})/(\text{volume of liquid})} \quad (25)$$

For non-particulate solids such as salt or granite whose permeability depends primarily on the extent of fracturing (secondary permeability) the selectivity coefficient was expressed by Borg et al. (1976) as

$$K_d(s) = \frac{\left\{ \begin{array}{l} \text{fraction in} \\ \text{solid phase} \end{array} \right\} \left\{ \begin{array}{l} \text{surface area} \\ \text{of solid} \end{array} \right\}}{\left\{ \begin{array}{l} \text{fraction in} \\ \text{liquid phase} \end{array} \right\} \left\{ \begin{array}{l} \text{volume of} \\ \text{liquid} \end{array} \right\}} \quad (26)$$

The differences in these equations reflect the importance of surface area in sorption phenomena. Sorption takes place at the surface of the solid, not penetrating more than a few molecular layers. Therefore, if all the other conditions remain constant, a larger surface area will increase the ion exchange capacity of a solid.

Selectivity coefficients, at least theoretically, can be calculated using the standard chemical mass-action equilibrium equation and laboratory results. Given a simple exchange equation such as:

Using the same terms as the mass-action equilibrium equation, the selectivity coefficient can be computed as:

$$K_d = \frac{(MX_m)}{(M^{+m})} = K_{m,a} \frac{(AX_a^m)}{(A^{+a})^m} \quad (28)$$

where

M^{+m} = concentration of M in solution in equivalents per unit volume

MX_m = concentration of M on the ion exchanger in equivalents per unit weight

A^{+a} = concentration of A in solution in equivalents per unit volume

AX_a = concentration of A on the ion exchanger in equivalents per unit weight

m, a = number of molecules

where

$K_{m,a}$ = mass-action equilibrium constant and is defined as

$$K_{m,a} = \frac{(MS_m)^a (A^{+a})^m}{(AX_a) (H^{+m})^a} \dots \dots \dots (29)$$

By measuring the concentration of the ion in solution and on the ion exchanger and by looking up in the Handbook of Chemistry and Physics or calculating the mass-action equilibrium constant, a theoretical selectivity coefficient can be calculated. Two major assumptions inherent in the mass-action equilibrium equation must be taken into consideration when using a selectivity coefficient that has been calculated from it. They are:

1. The mass-action equilibrium equation depicts conditions at equilibrium. In other words, it assumes that the time required to reach equilibrium is less than the rate of groundwater flow. Because the flow velocity in bedded salt deposits is so small, this is probably a valid assumption. However, this should be verified experimentally. Spitsyn and Balukova (1967) report that in the soil samples they tested, equilibrium was reached within 30 minutes to 8 hours.
2. The mass-action equilibrium equation only includes one cation or radioactive ion and one solid or mineral type. Such a simple situation would never exist in nature. Instead, several different radioactive ions would be competing for available exchange sites, which would probably include many different minerals.

Because of the many site specific factors that effect K_d values such as pH, brine concentration, bedding planes, fracture patterns, mineral composition, temperature, etc., K_d values need to be determined on-site. In practice, in-situ tests are seldom possible. Instead, samples are brought back to a laboratory and tested. A description of laboratory testing process can be found in Borg, et al. (1976), pages 151-152.

Methods that have been developed for calculating K_d values of several competing ions in solution with each other are described in Borg, et al. (1976), pages 142-148. They are all based on the mass-action equilibrium equation and the assumption "that the sum of all the equivalent concentrations of all the competing cations is equal to the total cation exchange capacity of the ion exchanger" or

$$Q = (AX_a) + (BX_b) + \dots + (MX_m) \dots \dots \dots (30)$$

where

Q = total cation exchange capacity

AX_a, BX_b, MX_m = equivalent cation concentrations

Although some researchers have gotten good K_d approximations based on calculations, particularly with the montmorillonite group (Borg, et al., 1976), the most accurate selectivity coefficients are determined experimentally.

The distribution coefficient table from Borg, et al. (1976) is shown below. It lists the K_d values found for rocks at the Nevada Test Site (NTS). Note that a wide range of values exists even between samples of the same rock type. The large variation reflects the lack of homogeneity in most formations, the sensitivity of the K_d value to different conditions and the problems inherent in measuring K_d values. Unfortunately, we were unable to find a specific K_d value for shale as a rock type which is known to have an extremely high adsorption capacity.

Sorption Equilibrium Constant

After the selectivity coefficient has been found, the ratio of the water velocity to the nuclide velocity, the sorption equilibrium constant, K , the value that is actually used in the computer model, can be found. For particulate media

$$V_i = \frac{V_w}{1 + K_d \rho \left(\frac{1 - \phi}{\phi} \right)} = \frac{V_w}{K} \dots \dots \dots (31)$$

where

K = sorption equilibrium constant

K_d = selectivity coefficient (ml/gm)

ρ = bulk density of medium (gm/cm³)

ϕ = porosity of medium

V_i = velocity of ion (cm/sec)

V_w = velocity of water (cm/sec) (Burkholder, et al., 1976)

For monolithic or non-particulate mediums such as salt or granite where secondary permeability predominates

$$K = 1 + K_d(s)R_f \dots \dots \dots (32)$$

where

R_f is the surface to volume ratio of the fault (Burkholder, et al., 1976)

So that for monolithic mediums

$$V_i = \frac{V_w}{1 + K_d(s)R_f} \dots \dots \dots (33)$$

Cation Exchange Capacity

The cation exchange capacity is a unique characteristic of the solid phase. According to Schwartz (1975), "Qualitatively the cation exchange capacity indicates the total amount of cations that can be exchanged under

DISTRIBUTION COEFFICIENTS (K_d) FOR NTS ROCKS AND OTHER NUCLEAR-EXPLOSIVE
MEDIA:^d STRONTIUM AND CESIUM.

Medium	K_d (ml/g)		Solution ^a	Sample Preparation ^a	Particle Size ^a	Time ^a (hours)	Notes	Reference
	Sr	Cs						
Alluvium, Central Nevada (Faultless)	48-2454	121-3165	Ground water	Ground	500-4000 μ m	96	Variation reflects different rock samples.	Nork et al. (1971)
Tuff, Rainier Mesa, NTS	260	1020	Prepared water	Ground	>400 μ m	72	Water to simulate Rainier Spring.	Nork and Fenske (1970)
Tuff, Rainier Mesa, NTS	2070-3480	12,100-17,800	Prepared water	Ground	100-200 mesh	168	Variation reflects variation in two rock samples. Solution closest to ground water.	Goldberg et. al. (1962)
Tuff, Rainier Mesa, NTS (Area 12b#2)	1700-4360	--	Prepared water	Ground	ng	168	Variation reflects different solutions. $C_{Ca} + C_{Mg} = 0.6-1.0$ meq/l; $C_{Na} = 0.1-2.0$ meq/l.	Kaufman (1963)
Tuff, NTS (Area 5)	400	5000-8000	Ground water	Chimney rubble	Chimney rubble	10 years	Values calculated from water sampling in partially filled chimney.	Hoffman (1975)
Tuff, NTS	4000	--	ng	ng	ng	ng		Stead (1964)
Carbonate, Yucca Flat, NTS	0.19	13.5	Prepared water	Ground	>4000 μ m	72	Water to simulate well water.	Nork and Fenske (1970)
Dolomite, Rustler Formation, New Mexico (Gnome)	5-14	--	Prepared water	ng	ng	ng	4250 ppm dissolved solids in water.	Stead (1963)
Granodiorite, Climax Stock, NTS (Hardhat and Piledriver)	4-9	8-9	Prepared water	Ground	100-200 mesh	72	Variation related to slight differences in prepared solutions, which were meant to simulate ground waters.	Beetem et. al. (1962)
	11-23	1030-1810	Prepared water	Crushed	0.5-1 mm	720		
Granite, Central Nevada (Shoal)	1.7	34.3	Deep formation water	Ground	>4000 μ m	720		Nork and Fenske (1970)
Basalt, Buckboard Mesa, NTS (Donny Boy)	16-135	792-9520	Prepared water	Ground	32-80 mesh	264	Variation due to solution differences; lower values representative of formation water.	Angelo et. al. (1962)
Pillow basalt, Amchitka, UAE-2 (1189 m)	220	39	Prepared water	Ground	500-4000 μ m	72	310 ppm dissolved solids in solution.	Essington and Nork (1969)
Basalt, Amchitka, UAE-3 (1741 m)	1220	280	Prepared water	Ground	500-4000 μ m	72	310 ppm dissolved solids in solution.	Essington and Nork (1969)
	1.1	6.5	Seawater	Ground	500-4000 μ m	72	310 ppm dissolved solids in solution.	
Shaley siltstone, New Mexico (Gasbuggy)	8.32	309	GB-2 well water	Ground	>4000 μ m	72		Nork and Fenske (1970)
Sandstone, New Mexico (Gasbuggy)	1.37	102	GB-2 well water	Ground	>4000 μ m	72		Nork and Fenske (1970)
Salt, Tatum Dome, Mississippi	0.19	0.027	Saturated salt water	Ground	>4000 μ m	72		Nork and Fenske (1970)

^ang = not given

a given set of conditions." Clay minerals have very high cation exchange capacities. Due to the presence of clay minerals in shale deposits that are interbedded with the salt, cation exchange could be the major attenuation process. In other words, most of the sorption described by the selectivity coefficient, K_d , will be from cation exchange on to the clay minerals that are found interbedded with salt deposits.

Cation exchange capacity is measured in terms of chemical equivalents of dissolved ions adsorbed per gram of exchanger at pH 7. Ion-exchange capacity depends on surface area, so that clays and zeolites have particularly high cation exchange capacities. The table below lists cation exchange capacities for some clay minerals and particulate formations. The cation-exchange capacity of halite as well as its K_d value is very low. Values shown in the Spitsyn and Balukova (1967) report indicate that clay adsorption capabilities are several orders of magnitude higher than those of sandstone or limestone which have much higher adsorption capabilities than salt.

DISSOLUTION AND PRECIPITATION

Process Definition

Dissolution is the process by which a solid is dissolved into a liquid. Through contact with water, the solid is broken down into its ionic components and dissolved into the liquid. Precipitation is the opposite of dissolution; it is the process by which ionized components in a liquid combine together to form a solid. The parameters and variables involved in dissolution and precipitation are described below.

<u>Parameters</u>	<u>Processes</u>	<u>Variables</u>
fracturing and faulting		temperature
- surface area	Dissolution	pressure
- spacing	Precipitation	brine concentration
solubility		flowrate - volume of water
dissolution rate		saturation level

CATION EXCHANGE CAPACITIES

Mineral or Rock	Capacity meq/g	No. of Samples	Mean Capacity meq.
Kaolinite ^{ab}	0.02 -0.10		
Muscovite ^{ab}	0.105		
Illite ^{ab}	0.13 -0.42		
Attapulgite ^{ab}	0.18 -0.22		
Nontronite ^{ab}	0.57 -0.64		
Saponite ^{ab}	0.69 -0.81		
Montmorillonite ^{ab}	0.8 -1.5		
Biotite ^{ab}	0.03		
Vermiculite ^{ab}	1.0 -1.5		
Upper Till ^c	0.22 -1.09	17	0.54
Middle Sand ^c	0.30 -0.69	7	0.50
Lower Till ^c	0.26 -0.86	8	0.52
Brown Silt ^c	0.57 -1.10	22	0.93
Cretaceous Shale ^c	0.35 -1.45	3	0.93

^aThese values are representative of a number of samples, but wide variations are possible for a given mineral depending upon its source and precise composition. In some cases where edge and corner exchange is appreciable, the capacity depends markedly upon particle size, e.g., kaolinite and illite; where exchange principally involves interlayer cations the effect of particle size is small.

^bClay mineral cation exchange capacity taken from Table 22 Borg, et al., 1976.

^cValues taken from Table III, Schwartz, 1977.

In this section we are interested in changes in the salt formation from the interstitial flow of groundwater. Flow through individual grains with dissolution on one side of the grain and precipitation on the other side of the grain due to thermal gradients is discussed in another section of this report.

Dissolution and precipitation are described in most introductory chemistry texts such as Pimental and Spratley (1971). Each solid chemical has a characteristic solubility in water at a given temperature and pressure. The solubility is the number of grams that can be dissolved per liter of the solute (water). When the amount of solute in solution has reached solubility, the solution is said to be saturated or to have reached its equilibrium. For a detailed, theoretical discussion of dissolution, see a chemistry text such as Pimental-Spratley (1971).

The solubility or saturation level of a given solution increases with increasing temperature. The table below gives the solubilities for pure NaCl in pure water at atmospheric pressure for a few obscure temperatures.

NaCl SOLUBILITY

356,484 mg/l	in 25°C water (Pimental & Spratley)
357,000 mg/l	in cold water (CRC Handbook)
391,200 mg/l	in hot water (CRC Handbook)

In a typical groundwater with dissolved solids, the solubility of salt would be different from the values listed in the above table.

Because the chemical composition of groundwaters and salt deposits are complicated, their solubilities at various temperatures will have to be determined experimentally and cannot be based on tables for pure chemicals.

Saturation levels also vary slightly with changes in pressure. The range of pressures considered in the bedded salt deposits, however, will not cause any significant difference in saturation level.

The solubility tells you the amount of salt that can be dissolved, but not the rate at which it dissolves. In general, however, compounds with high solubilities dissolve quickly. The rate of dissolution is directly related to the surface area of the solid exposed to the liquid. For example, a solid halite cube would dissolve much more slowly than the same mass of halite in powder form.

As Claiborne and Gera (1974) explain, the change in mass of a cube with time can be expressed as

$$\frac{dm}{dt} = -3a^2\ell \quad \dots \dots \dots (34)$$

for

$$m = a^3\rho \quad \dots \dots \dots (35)$$

where

- m = mass
- t = time, days
- a = length of cube side, cm
- ℓ = leach rate, g/cm²-day
- ρ = density of particle, g/cm³

In the case of groundwater flow through a fractured salt deposit, "a" will equal the average distance between joints. The leach rate will be a function of the groundwater flowrate with the volume of water limiting the amount of salt that can be dissolved. Because the solubility of salt is so high and the rate of groundwater flow so small, it can be assumed that all fresh water that comes in contact with the salt will immediately become saturated (Claiborne and Gera, 1974). If the amount of fresh water that will come in contact with the salt is known, the amount of salt dissolved can be calculated, so that :

$$\left[\begin{array}{c} \text{solubility} \\ (\text{mg/l}) \end{array} \right] \times \left[\begin{array}{c} \text{volume of groundwater} \\ (\text{liters}) \end{array} \right] = \begin{array}{c} \text{salt dissolved} \\ (\text{mg}) \end{array} \quad \dots (36)$$

If the brine moves through areas of different temperatures, the saturation level of the solution will change. As the temperature drops, the saturation level drops and precipitation will occur. When groundwater moves away from heated zones, salt crystals will be precipitated onto the fracture faces reducing the size of the flow channels.

Natural Dissolution

Based on the amount of salt dissolved by surface waters, Swenson (1974) has calculated the approximate rate of salt dissolution for several subbasins draining the Permian Basin. These rates are listed in the table below. Even at the highest dissolution rate calculated, only 0.5 ft of salt would be dissolved in 1,000 years if the dissolution was spread evenly throughout the subbasin.

The fact that salt beds have survived for more than 250 million years indicates their ability to repel groundwater and withstand dissolution. The tight seal of the impermeable shale that generally surrounds salt beds has undoubtedly been their major protection from groundwater.

DISSOLUTION RATES IN PERMIAN BASIN (SWENSON, 1974)

Subbasin	Dissolution Rate	Year
Reach of Salt Fork of Brazos River	967 tons/mi ² -yr 955	Average 1966
Colorado River above Ira, Texas	17 tons/mi ² -yr	-
Colorado River between Ira and Colorado City	60 tons/mi ² -yr	-
Trinity River	18 tons/mi ² -yr	-
Lake Texamo of Red River	126 ton/mi ² -yr	-
Walnut River	33 tons/mi ² -yr*	1966

* Half of sodium chloride content from past brine disposal.

THERMAL RELATED PROCESSES

Process Definition

Water in geologic formations is in motion. Several types of gradients may be involved in this motion including hydraulic pressures, density induced, and geothermal gradients. In thick aquifer/aquitard systems, interaction of these gradients induce gravity convection currents which may cause entrained wastes to migrate in unanticipated directions. A particularly enlightening article by Henry and Kohout (1972) discusses water circulation patterns affected by geothermal potential gradients related to disposal of liquid waste in deep saline aquifers.

This report section discusses the geothermal processes related to groundwater motion. Since many groundwater parameters, such as density and viscosity, are temperature-dependent, one must realize that there is a great deal of coupling with other processes described in this report.

According to Bear (1972), heat is transported in a fluid-porous medium by the three modes: conduction, convection, and radiation. "Conduction" is the mechanism of thermal energy exchange due to the exchange of kinetic energy among colliding molecules, yet without appreciable displacement of the latter. "Convection" is the mechanism of the thermal energy transport in fluids associated with the actual mass movement of fluids from one region to another. Convection imposed by external means is known as forced convection, while fluid motion caused by density difference due to temperature variations in the field of flow is called free or natural convection. "Radiation" is essentially a mechanism of emission of electromagnetic waves that allows energy to be transported with the speed of light through regions of space that are devoid of any matter.

In a porous medium whose void space is filled with a moving fluid, the three basic modes of heat transfer manifest themselves in the six following ways:

1. Heat transfer through solids by conduction.
2. Heat transfer through fluids by conduction.
3. Heat transfer through fluids by convection.
4. Heat transfer through fluid/solid matrix by dispersion (completely analogous to hydrodynamic dispersion discussed in "Dispersion and Diffusion" section of this report).
5. Heat transfer between the solid and fluid phase by conduction.
6. Heat transfer between solid grains by radiation when the fluid is a gas.

The heat transfers of concern here involve the entire sequence of geologic formations including all aquifers, aquitards, and aquicludes of Figure 1.

As a beginning, the parameters and variables involved in this process are as shown below:

<u>Parameters</u>	<u>Process</u>	<u>Variables</u>
specific heat of fluid		velocity
specific heat of solid/ fluid complex		temperature
density of fluid	Heat and	pressure
density of solid/fluid complex	Mass Transport	time
thermal conductivity of solid/fluid complex		
porosity of solid		
viscosity of fluid		
coefficient of thermal dispersion		

Mathematically, the general differential equation for one-dimensional unsteady heat and fluid flow through isotropic, homogenous, and fully saturated porous media is (Stallman, 1963):

$$\frac{\partial^2 T}{\partial x^2} - \frac{c_0 \rho_0}{k} \frac{\partial (v_x T)}{\partial x} = \frac{c_0}{k} \frac{\partial T}{\partial t} \dots \dots \dots (37)$$

where

- T = temperature at any point at time t (C)
- c₀ = specific heat of fluid (cal/g- C)
- ρ₀ = density of fluid (g/cm³)

c = specific heat of solid/fluid complex (cal/g-°C)
 ρ = density of solid/fluid complex (g/cm³)
 k = thermal conductivity of solid/fluid complex (cal/cm-sec-°C)
 v_x = component of fluid velocity in x direction (cm/sec)
 X = cartesian coordinate
 t = time since flow started (sec)

The parameter list above includes viscosity and porosity which are not directly in the above equation. These two parameters fit within the velocity term, v_x , as was discussed in the "Advection Process" section of this report. Reference should be made to that section for ranges of values of viscosity and porosity. In addition, one should refer to the water density table given in the "Advection Process" section. The remaining parameters above are discussed below.

Specific Heats of Fluid, Solid, and Solid/Fluid Complex

In the context used in this report, specific heat--or more properly--the thermal capacity of a substance is defined as the quantity of heat (calories) necessary to raise the temperature of a mass (grams) of the substance one degree celsius.

Numerous tables are available on values of specific heats of solids and fluids. An abbreviated table of specific heat of water taken from the Handbook of Chemistry and Physics (1970) is given below.

Temperature C	Specific Heat of Water (cal/g-°C)
0	1.00738
10	1.00129
20	0.99883
30	0.99802
40	0.99804
50	0.99854
60	0.99943
70	1.00067
80	1.00229
90	1.00437
100	1.00697

Bear (1972) gives specific heat values for various dry rocks as follows:

Dry Rock Material	Temperature °C	Specific Heat (cal/g-°C)
Basalt	20 - 100	0.20
Chalk	20 - 100	0.214
Clay	20 - 100	0.22
Granite	12 - 100	0.192
Quartz	12 - 100	0.188

Other values of specific heat from Carslaw and Jaeger (1959) were given as rough averages below.

Substance	Specific Heat (cal/g-°C)
Limestone	0.22
Sandstone	0.23
Soil (average)	0.20
Soil (sandy, dry)	0.19

Dames and Moore (1970) give the following specific heats for the following salt-type materials:

Material	Specific Heat (cal/g-°C)
Halite (intact salt)	0.19 to .47
Salina salt	0.22
New Mexico potash - rich rock salt	0.22
Kansas salt	0.22
Generic salt	0.20 @ 0 C 0.21 @ 100 C 0.22 @ 200 C

It may be of interest to note that the specific heat values above are very nearly alike for all of the solid materials--namely, approximately 0.21 cal/g-°C. Dames and Moore quote Gera's (1972) specific heat of 0.47 for the intact salt in the list above. We would suggest a thorough investigation of this high value before using it for any purpose.

Bear (1972) further lists specific heats of some selected gases as follows:

Gas Type	Temperature °C	Specific Heat (cal/g-°C)
Air	50 (20 atm)	0.2480
Water vapor	100	0.4820
Oxygen	15	0.2178
Methane	15	0.5284

The combination of parameters c_p of Equation (37) above is sometimes called the effective heat capacity of the solid/fluid complex.

This effective heat capacity term, c_e , may be calculated for the various solid/fluid pairs from the following equation from Bear (1972):

$$c_e = c_p = \eta \rho_f c_f + (1 - \eta) \rho_s c_s \quad \dots \dots \dots (38)$$

where

- η = porosity of solid
- ρ = density of fluid (g/cm³)
- c = specific heat of fluid (cal/g-°C)
- ρ_s = density of solid (g/cm³)
- c_s = specific heat of solid (cal/g-°C)

Values of water densities and porosities are given in the advective transport section of this report, and c_f and c_s values are given above. Typical density values of solids taken from Carslaw and Jaeger (1959) and Dames and Moore (1973), and the Handbook of Chemistry and Physics (1970) are as follows:

Material	Density (g/cm ³)	Reference
Basalt	2.4 - 3.1	Handbook of Chemistry and Physics (1970)
Chalk	1.9 - 2.8	" "
Clay	1.8 - 2.6	" "
Coal, anthracite	1.4 - 1.8	" "
Coal, bituminous	1.2 - 1.5	" "
Dolomite	2.84	" "
Granite	2.64 - 2.76	" "
Limestone	2.68 - 2.76	" "
Quartz	2.65	" "
Rock salt	2.18	" "
Sandstone	2.14 - 2.36	" "
Soil (average)	2.5	Carslaw and Jaeger (1959)
Soil (sandy, dry)	1.65	" "
Air	0.00129	" "
Rock salt	2.03 - 2.44	Dames and Moore (1973)

Thermal Conductivity of Fluid, Solid, and Solid/Fluid Complex

The thermal conductivity of a substance is the proportionality constant relating the time rate of transfer of heat by conduction, through unit thickness, across unit area for unit difference of temperature. The dimension of thermal conductivity is cal/cm-sec - °C.

A table of thermal conductivities is listed below for both liquids, solids and gases. The values given from Carslaw and Jaeger (1959) and Bear (1972) are listed for order of magnitude only since thermal conductivity is a function of temperature. Where temperature versus thermal conductivity values are available, they are listed.

Material	Temperature °C	Thermal Conductivity (cal/cm-sec-°C)	Reference
NaCl		0.008 - .015	Bear (1972)
Sandstone		0.009	" "
Limestone		0.005	" "
Dolomite		0.004 - 0.01	" "
Clay		0.002 - .003	" "
Water		0.0011	" "
NaCl (25%) solution		0.000138	" "
Petroleum		0.00035	" "
Air		0.00006	" "
Generic salt	0	0.0146	Dames and Moore (1978)
	50	.0120	" "
	100	.0100	" "
	150	.0086	" "
	200	.0074	" "
	250	.0066	" "
	300	.0059	" "
	350	.0055	" "
	400	.0050	" "
Granite		.0045 - .0096	Handbook of Chemistry & Physics (1970)
Average rock		.0042	Carslaw and Jaeger (1959)
Soil (average)		.0023	" "
Soil (sandy, dry)		.00063	" "

According to Bear (1972), the thermal conductivity used in Equation (37) above, must be the equivalent fluid/solid conductivity. The tables above are for various dry solids and fluids separately. Bear (1972) gives the following equation to calculate an equivalent thermal conductivity which is the parameter k (thermal conductivity of fluid/solid complex) of Equation (37):

$$k = \eta k_f + (1 - \eta) k_s \quad \dots \dots \dots (39)$$

where

η = porosity

k_f = thermal conductivity of fluid (cal/cm-sec C)

k_s = thermal conductivity of solid (cal/cm-sec C)

In actuality, there are other formulas for calculating equivalent thermal conductivities (see Bear, 1972). However, all formulas suggested manipulate the same parameters of Equation (39).

Coefficient of Thermal Dispersion

Equation (37) could have included a term including thermal coefficient of dispersion (similar to mechanical hydrodynamic dispersion mentioned in the Dispersion and Diffusion section of this report). This term would take on the form of:

$$\frac{\partial}{\partial x} \left(D_{\text{therm}} \frac{\partial T}{\partial x} \right) \quad \dots \dots \dots (40)$$

which expresses the dispersive heat flux and where

D_{therm} = coefficient of thermal dispersion

As pointed out by Green (1963), and on the basis of available data, the D_{therm} and the hydrodynamic dispersion coefficient are practically

identical up to a Peclet number of 10^4 . A Peclet number is a dimensionless coefficient which incorporates heat capacity, density, and fluid velocity and is used to determine the chemical scale-up similitude for scale-up from pilot plant data to commercial size units. Moreover, the coefficient of thermal dispersion is negligible as compared with the conductive one when the Peclet number is less than 3,000 (which corresponds approximately to the Darcian range). This implies that the hydrodynamic dispersion coefficients listed elsewhere in this report can be used for the thermal dispersion coefficient when appropriate; and altogether neglected where appropriate for Darcian laminar flow range.

One should not forget that the process of hydrodynamic dispersion is taking place along with the thermal process as it relates to changes in pressure and density. Reference is made to the section on dispersion and diffusion to note this set of parameters.

THERMOMIGRATION

According to Anthony and Cline (1974), typical salt formations contain about 0.4 percent water trapped in tiny pockets. Furthermore, and as stated by Cohen (1977), "The solubility of salt in water increases with temperature, so that if the temperature on one side of the pocket is raised, more salt will go into solution on that side. This raises the salt content of the water above the saturation point for the temperature on the opposite side of the pocket, however, causing the salt to precipitate out of solution on that side. The net effect is a migration of the water pocket in the direction of the higher temperature," (which is the direction of the buried wastes).

This thermomigration process is expected to lead to the collection of water near the canisters of the repository. Since the temperature at the surface of the canister would be higher than the boiling point of water, steam would be produced consisting of brine water vapor. It is

a possible result of the self-heating of the nuclear wastes that contaminated vapor-liquid biphasic droplets generated on the walls of the repository may transport radioactive wastes away from the repository into the salt formation. According to Anthony and Cline (1974), the temperature gradient likely to exist may cause the vapor-liquid droplets, containing only vapor in the vapor phase, to carry nuclear wastes only a distance of 600 centimeters into the salt formation in two years. However, Anthony and Cline further point out that their distance calculation ignores the ability of salt grain boundaries to trap migrating droplets.

Anthony and Cline (1974) concluded that an inflow of water into the nuclear repository can be expected and that dispersal of radioactive wastes into the salt formation may occur. However, because grain boundaries in salt can trap migrating droplets, it is unlikely that radioactivity will escape to the external environment even on a geological time scale.

The conclusions we have come to concerning thermomigration processes are that they are local in effect. Any radioactive release from such a process would thus, for our regional view, be a boundary condition. Once the wastes are within the salt, further transport would thus be accounted for by the other processes discussed elsewhere in this report.

RADIOACTIVE DECAY PROCESS

According to Schwartz (1975), one of the most important nuclear processes to be considered in radioactive-contaminant migration is the influence of radioactive decay. This process is a natural attenuation mechanism. The change in concentration of the radioactive materials is described mathematically as:

$$\frac{dC}{dt} = -\lambda C \quad \dots \dots \dots (41);$$

where

T = time

C = concentration

λ = positive rate constant

The solution of the equation is

$$C = C_0 e^{-\lambda t} \dots \dots \dots (42)$$

where C_0 is the initial concentration. The time required for the concentration C to decrease to one-half the initial concentration C_0 is defined as the half-life of the substance. Schwartz continues by showing that there is a simple relationship between the half-life and the radioactive constant λ . By substituting $C = C_0/2$ in the above equation and solving for λ , the following relationship is obtained:

$$\lambda = \frac{\ln 2}{t_{1/2}} = \frac{0.693}{t_{1/2}} \dots \dots \dots (43)$$

where

$t_{1/2}$ = half-life

Ordinarily, the radioactive decay process equation is added to a dispersion equation to give, for example:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial C}{\partial x} \right) - V \frac{\partial C}{\partial x} - \lambda C \dots \dots \dots (44)$$

This is a one-dimensional dispersion-advection equation governing the mass transport of a fluid species undergoing radioactive decay through a porous medium. C , D , and V in the above equation are the fluid concentration, dispersion coefficient, and velocity respectively (see sections on Dispersion and Diffusion for dispersion parameters).

The parameter of prime interest here is the half-life. In terms of waste management, radioactive materials with longer half-lives pose the most serious problem because subsurface confinement must be sufficient to allow decomposition through several half-lives. A table is given below of half-lives of selected radioisotopes. The half-life parameter values below were taken from the Handbook of Chemistry and Physics (1970).

Isotope	Half-Life (Years)
Sr 90	28.1
Tc 99	2.12×10^5
Cs 137	$30.23 \pm .16$
Sm 151	$93 \pm 8^{**}$
Eu 154	15
Pu 238	86
Pu 239	24,400
Pu 240	6,580
Pu 241	13.2
Am 241	458
Cm 244	17.6
I 129	1.7×10^7
N_p 237	2.14×10^6

Parameter Uncertainties

The previous sections of this report described eight major processes that should be included in a model of regional radionuclide waste migration in bedded salt formations. To model these processes, 26 parameters must be known or estimated. These parameters are listed in the following table. In addition to the parameter list, we have also included a qualitative assessment of how well the parameter values are known. This qualitative ranking, in order of certainty, is:

- Well known
- Needs improvement
- Uncertain
- Highly uncertain
- Unknown

Of the 26 parameters, only eight are considered to be well known, while seven need improvement. The remaining eleven parameters are in various categories of uncertainty. These are parameters that should receive special attention in future research efforts.

PARAMETER SUMMARY

Parameter	Value Certainty
Diffusion coefficient	Needs improvement
Dispersion coefficient	Uncertain
Specific permeability	Highly uncertain
Viscosity	Well known
Specific weight	Needs improvement
Porosity	Uncertain
Specific yield	Unknown
Dispersivity constant	Highly uncertain
Rock strength	Well known
Radiation level	Well known
Bulk density	Well known
Void fraction	Needs improvement
Cation exchange capacity	Uncertain
Selectivity coefficient	Highly uncertain
Sorption equilibrium constant	Highly uncertain
Surface area	Unknown
Spacing of fractures	Unknown
Solubility	Needs improvement
Dissolution rate	Needs improvement
Specific heat of fluid	Well known
Specific heat of solid/fluid complex	Needs improvement
Density of fluid	Well known
Density of solid/fluid complex	Well known
Thermal conductivity of solid/fluid complex	Needs improvement
Coefficient of thermal dispersion	Uncertain
Radioactive decay rate	Well known

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