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Panel Report
on
Coupled Thermo-Mechanical-Hydro-Chemical Processes Associated with a Nuclear Waste Repository

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PANEL ON COUPLED PROCESSES
ASSOCIATED WITH GEOLOGICAL DISPOSAL OF NUCLEAR WASTE

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INTRODUCTION

Background of this Study

The assessment of the long-term performance of a nuclear waste repository involves the evaluation of the travel time and rate of transport of radioactive elements from the repository to the accessible environment. This evaluation involves understanding the combined effects of many different processes that may affect such transport. A study was initiated with the recognition of the need to have a multidisciplinary study of the coupled physical and chemical interactions in geological systems involving heat transfer, ground water hydrology, geomechanics and geochemistry that will increase our understanding of the important processes affecting the long term performance of a nuclear waste repository. The focus of this study is to identify systematically which coupled interactions are important for different geologic media. The project goals are: (1) identifying a list of coupled processes, (2) evaluating these processes according to their importance for the long term performance of the repository, insofar as this is possible with our current state of knowledge, (3) ranking these processes according to the uncertainties involved, and (4) suggesting possible approaches that might be taken to study these processes to reduce uncertainties and resolve key issues. Published information on hydrothermal systems and other natural water/rock systems that have experienced conditions similar to those anticipated around a repository will be identified. In this way the foregoing issues may be better addressed and a clearer understanding obtained of whether and under what conditions the various coupled interactions are important for the geological disposal of nuclear waste.

To facilitate this study a Panel of experts was selected composed of scientists representing the disciplines of ground water hydrology, rock mechanics and geochemistry (see Panel membership list). The Panel is to meet annually during the three years (FY 1984-86) of this project. This Panel Report is from the first of these meetings, held on January 25-27, 1984, at Lawrence Berkeley Laboratory. Therefore, the discussions and conclusions are preliminary and tentative in nature. They will be re-evaluated at the next two meetings based on new research results from various ongoing projects and information collected from hydrothermal and related fields. Any comments and suggestions in response to this Report are welcomed, and should be directed to the Panel Chairman, Paul A. Witherspoon or to Chin-Fu Tsang.

Coupled Processes

The investigation of the predicted performance of a nuclear waste repository requires a comprehensive view of the major physical processes likely to occur. The major processes are Thermal (T), Hydrological (H), Mechanical (M), and Chemical (C). Among these four categories of processes there can be only 11 (i.e., $2^4 - 5$) types of couplings of various degrees of importance. They are summarized in Table I.

In the course of the first panel meeting, we found it useful to draw definite distinctions between different degrees of coupling in order to clarify what we mean by coupled and uncoupled processes. Table II displays schematically several possible connections between processes. The fully uncoupled processes conceptually have negligible influence or effect on one another, so that they can be evaluated independently. The sequential case implies that one process depends on the final state of another so that the order in which they are evaluated becomes important.

The one-way coupled processes demonstrate a continuing effect of one or more processes on the others, so that their mutual influences change over time. The two-way coupling (or feedback coupling) reveals a continuing reciprocal interaction among different processes, and represents in general the most complex form of coupling. In this study, the term coupled processes refers to either the one-way or the two (or more)-way couplings among the physical processes considered.

At its first meeting, the Panel discussed various coupled processes, their importance and uncertainties. A list of the coupled processes that were identified and discussed is given in Table III. In what follows, the discussions by the Panel members are summarized in three sections: (1) coupled chemical processes (geochemistry), (2) coupled fluid dynamics processes (groundwater hydrology), and (3) coupled mechanical processes (rock mechanics). Each section is preceded by a table of contents. The sections were written by different Panel members in their respective areas of expertise, and, except for some editing and rearranging, the style and manner of presentation has been left according to their own contributions.

Following the Panel discussions is a section composed of a series of tables where the various processes considered are tentatively evaluated according to their significance and the uncertainty of our knowledge concerning them, plus some additional comments concerning ways in which they may be investigated. These tables were derived from verbal discussions during the three-day meeting of the Panel, so they should be taken as only a preliminary estimate of the ranking of the processes involved. The ranking is classified qualitatively according to H = High, M = Medium and L = Low, but for most processes in the tables the rankings are high because discussion was centered on processes which are likely to be most significant for repository performance, and therefore only a few processes of low importance were considered. The tables are useful mainly as an overall checklist to ensure that no significant coupling has been overlooked, rather than as an established priority list. These lists and their priorities will no doubt be modified and improved during the next two Panel meetings.

It should be emphasized that this evaluation of the significance of the coupled processes was done from a general perspective. For any specific site the relative rankings of H, M, or L may be quite different depending on the characteristics of the particular site; it is well known that geologically each site is unique. Thus, we also should consider these processes in the context of the geological systems of interest. For disposal of nuclear waste, four major geological systems have been widely discussed with some relevant characteristics summarized in Table IV. This Table along with Table I may provide a general framework for the following discussion.

Table I

Types of Coupled Processes

(T = Thermal, M = Mechanical, H = Hydrological, C = Chemical;
single line indicates weak coupling, double line, strong coupling)

	Type	Examples
1.	T═C	e.g. phase changes
2.	T═H	e.g. buoyancy flow
3.	T═M	e.g. thermally induced fractures
4.	H═C	e.g. solution and precipitation
5.	H═M	e.g. hydraulic fracturing
6.	C—M	e.g. stress corrosion
7.		e.g. chemical reactions and transport in hydrothermal systems
8.		e.g. thermomechanical effects with change of mechanical strengths due to thermochemical transformation
9.		e.g. thermally induced hydromechanical behavior of fractured rocks
10.		e.g. hydromechanical effects in fractures that may influence chemical transport
11.		e.g. chemical reactions and transport in fractures under thermal and hydraulic loading

Table II

Diagrams of Uncoupled and Coupled Processes

(T = Thermal, M = Mechanical, H = Hydrological, C = Chemical)

Uncoupled Processes

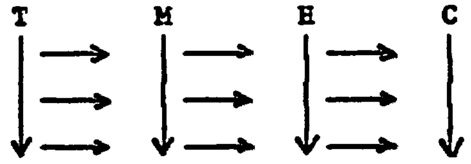
Fully Uncoupled

Sequential, e.g.

T → M → H → C →

Coupled Processes

One-way Coupling, e. g.



Two-way Coupling, e. g.
(Feedback Coupling)

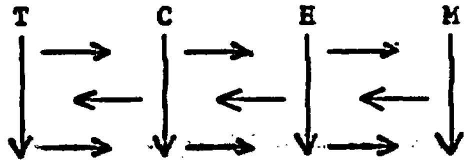


Table III

List of Coupled Processes

I. Thermochemical (TC)

- Thermal Diffusion
- Phase Changes--Equation of State of Solids
- Solid Solution
- Metastable Phases

II. Thermohydrological (TH)

- Convection Currents (1 or 2 phases) including Buoyancy Flow
- Phase Changes and Interference
- Thermophysical Property Changes
- Thermal Osmosis
- Gas Diffusion:
  - Binary
  - Knudsen
  - Thermal
  - Coupled
- Capillary - Adsorption

III. Thermomechanical (TM)

- Induced Cracking
- Fracture Deformation
- Thermal Spalling
- Thermal Creep
- Thermal Expansion

IV. Hydrochemical (HC)

- Speciation
- Complexation
- Solution
- Deposition
- Sorption/Desorption
- Redox Reactions
- Complexation
- Hydrolysis
- Acid - Base Reactions
- Diffusion
- Chemical Osmosis and Ultrafiltration
- Isotopic Exchange
- Coprecipitation

Table III (continued)

V. Hydromechanical (HM)

- Hydraulic Fracturing
- Pore Pressure Change
- Hydraulic Erosion of Fractures
- Sedimentation of Particles
- Shear Effect Causing Abrasion
- Variation of Fracture Apertures
- Filtration of Particles
- Ultrafiltration

VI. Mechanical-Chemical (MC)

These processes will be modified by hydrological and thermal effects, so they are included in processes VII and VIII below.

VII. Thermohydrochemical (THC)

- Solution/Precipitation
- Time-Dependent Solution and Precipitation
- Fluid Transport by Osmotic Effect
- Chemical Transport in Gas Phase
- Partition between Gas and Solid
- Particle Transport (Colloids)
- Equation of State
- Thermal Diffusion (Soret Effect)
- Thermal Osmosis

VIII. Thermomechanical-Chemical (TMC)

- Phase Change in Mineral Phases
- Dehydration
- Creep
- Hydration and Swelling

IX. Thermohydromechanical (THM)

- Hydraulic Fracturing
- Triggering of Latent Seismicity
  - Stress Redistribution
  - Pore Pressure
- Opening and Closing of Joints
  - Stress Redistribution
  - Thermal Coupling
  - Pore Pressure
- Spalling
- Change of Strength
  - Stress Corrosion
  - Hydrolitic Weakening
- Hydration

Table III (continued)

X. Hydromechanical-Chemical (HMC)

These processes were eliminated from consideration because without thermal effects the mass transport is not sufficient to change the geometry except for low temperature precipitation, pressure solution, and ion exchange producing swelling (e.g. Na for Ca in Smectites) at approximately 50°C or below.

XI. Thermohydromechanical-Chemical (THMC)

- Piping--Selected Dissolution and Tunnel Corrosion,
  Inhomogeneous Leaching
- Precipitation
  - In Fractures
  - In Matrix
- Hydrothermal Alteration of Rock
- Heat Pipe Effect with Dissolution/Precipitation
- Vertical Vapor-Liquid Cycling Near Canisters
- Pressure Solution

Table IV

Geological Systems

Formations	Outstanding Features
Tuff	Partially saturated High porosity Fractured-porous Low thermal conductivity
Basalt	Saturated Fractured-porous High permeability High sorbing and reducing capability
Salt (Bedded and Domed)	Low permeability High thermal conductivity Homogeneity Plasticity and creep
Granitic Rocks	Saturated Structural stability Chemically stable Low porosity and permeability Fractured

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Regions of Interest:	Near Field Far Field
Subsurface fluids:	Water Steam-water Air-steam-water

DISCUSSION ON COUPLED CHEMICAL PROCESSES:

Key Issues and Significant Uncertainties

Summary

Many coupled and uncoupled geochemical processes that can control the mobility of radionuclides from a breached repository are not adequately understood. Mobilization of radionuclides and related substances in ground water may occur by dissolution, desorption or colloidal deflocculation. Transport may carried out by advection, diffusion, membrane transport, or polymer-colloidal movement. Deposition may occur by precipitation or coprecipitation, adsorption, filtration, and flocculation and settling of colloids. Most of these processes cannot be rigorously understood without adequate thermodynamic and kinetic data bases. Empirically derived thermodynamic and kinetic data for radionuclides and related substances are largely lacking above 25°C and 1 bar pressure, although in some cases sufficiently accurate estimates of such data are now possible. Computer programs that can evaluate the status of reactions in water-rock systems as well as predict such reactions are available. Such programs and data bases are essential to define ground water conditions prior to repository siting and to predict repository performance after emplacement of waste.

Perhaps the most important coupled thermochemical process that can occur near a repository is the precipitation of secondary minerals. Studies using granite have shown that silica leached from the rock near a canister will precipitate at some distance away at lower temperatures, clogging pore space in the rock. At the same time minerals with retrograde solubility such as calcite and anhydrite are likely to precipitate on canister walls and may inhibit corrosion of the canister. Research quantifying these processes for the several rock types under repository conditions is needed.

Background water-rock conditions and the degree of isolation of the water-rock system must be known for potential repository sites. Such information can be gained through a combination of methods including age dating of the water using Cl-36 and isotopes of He, Ne and Ar; measuring stable oxygen and hydogen isotopes in the water; and modeling the status of water-rock reactions with computer codes such as WATEQ and PHREEQE.

The composition of backfill around a canister can be designed to minimize migration of radionuclides from a breached canister and to retard canister corrosion. This can be accomplished in part by enhancing the precipitation of silicates in pore spaces at a distance from the canister and the precipitation of carbonates and sulfates on canister walls. Other compositional designs can be used to reverse chemical potential gradients so that radionuclides will migrate toward rather than away from the canister.

Numerical simulation by digital computers will be required to assess coupled thermochemical and thermohydrochemcial processes in repository environments. Valuable insight into the evolution of systems including these processes can be gained by study and simulation of natural hydrothermal systems that can be used as analogs of a repository.

1. Introduction

When one considers the geochemical and related problems associated with the disposal of high level nuclear wastes in rocks including tuff, dome and bedded salt, basalt and granite, it becomes clear that numerous coupled and uncoupled geochemical processes that must be understood to ensure the safe disposal of the wastes are not understood. Table V is a schematic general statement of the processes that mobilize radionuclides and other minor and major elements, that transport these elements, and that lead to their deposition. The diagram applies to the mobilization of elements from a breached canister and their deposition in backfill materials, as well as to their mobilization, transport and deposition in surrounding geological media. The transport process will generally (but not always) be via an aqueous phase (i.e. ground water). Except for radioactive decay occurring within a solid phase, an understanding of all the processes listed always demands an understanding of their coupling with the hydrology or fluid dynamics of the ground water system.

Whether and how a major element species or trace radionuclide is mobilized, transported and deposited, depends on the thermodynamic properties of the aqueous species and solid phases involved, and also on the rates of the reactions among those aqueous species and solids.

2. The Thermodynamic Data Base

Thermodynamic data for most rock forming minerals is available for 25°C, and also for temperatures well above 250°C, the maximum temperature thought likely in a repository adjacent to the waste (see Robie and others, 1978).

Table V

Mechanisms of Mobilization, Transport and Deposition of Radionuclides and Other Chemical Substances in Ground Water-Rock Systems

Mobilization	Transport	Deposition
dissolution desorption deflocculation	advection, membrane transport, diffusion, polymer-colloidal transport	precipitation & coprecipitation adsorption filtration settling

Similar data have been published (in large part estimated) for major electrolyte species and some minor elements in relatively dilute solutions (c.f. Helgeson and others, 1981; and Arnorsson and others, 1982). However, comparable thermodynamic data for trace elements and especially for most radionuclides is lacking. Such data as exists for radionuclide solutes and minerals is generally for 25°C only, and must be estimated for elevated temperatures and pressures. Other major problems with the radionuclide thermodynamic data include the facts that much of the tabulated data is either inaccurate or internally inconsistent, and that important aqueous species or minerals have not been considered.

A number of researchers have addressed these problems, and have attempted to estimate thermodynamic properties for potentially important substances (c.f. Langmuir, 1978; Langmuir and Herman, 1980; Phillips, 1982; Phillips and Sylvester, 1983; Edelstein and others, 1982; Krupka and others, 1983; Phillips and others, 1984). The empirical data from which to calculate thermodynamic properties of the radionuclides and related species at elevated temperatures is usually unavailable. However, extension of a recently recognized generalization regarding reaction heat capacities (Murray and Cobble, 1980; Cobble and others, 1982) may make it unnecessary to obtain such high temperature empirical data for many reactions. For example, it has been observed that for reactions such as

$$BaSO_4(c) + Ra^{2+} = RaSO_4(c) + Ba^{2+}$$

$$HCO_3^- = OH^- + CO_2(aq)$$

where equal ion charges occur on both sides of the equation, the heat capacity of the reaction will remain nearly constant above 25°. Estimation of the thermodynamic properties of ionic species above 25°C by other methods, including the correspondence principle of Criss and Cobble (1961) based on measured or estimated entropies at 25°C, are often unreliable above 100°C.

Major thermodynamic data needs are: 1) reliable thermodynamic data for many radionuclide aquo-complexes at 25°C and above; 2) thermodynamic data for radionuclide solid solutions in major rock forming minerals (a likely fate via coprecipitation of, for example, Ra and Sr-90); and 3) thermodynamic data for the exotic metastable minerals including alumino-silicates phases likely to form adjacent to the canister and backfill at the elevated temperatures of the repository. These phases need to be identified experimentally as well as characterized thermodynamically.

It must be emphasized that the inadequacies in our thermodynamic data base are far less serious at 100°C than at 250°C. This in itself is an argument for reconsidering our choice of the maximum repository temperature, perhaps deciding as the Europeans have, that a maximum temperature of 80-100°C is desirable.

3. The Kinetic Data Base and Non-Equilibrium Processes

Although the thermochemical properties of aqueous species and minerals can provide a basis for predicting the limiting conditions to be expected in subsurface environments given sufficient time, many reactions important to high level nuclear waste disposal are either kinetically inhibited, or tend towards product species that are not simply predicted from the thermochemical data. For example, adsorption of Pu can be practically irreversible, and the high temperature dissolution of a clay backfill and of alumino-silicate country rock is likely to be an incongruent process, leading to the precipitation of such phases as zeolites and relatively amorphous mixed metal oxyhydroxides. Kinetics and the irreversibility of reactions is most important under near field conditions where thermal and chemical gradients are pronounced.

Radioactive decay rates are generally well known, however, rates of most other reactions for anticipated near field and far field conditions are not. In terms of repository performance prediction and uncertainty, the most important of these rates are the slowest. Rates which have half-lives of years or longer most need to be studied and understood. At temperatures below 50-100°C rates of many redox and precipitation-dissolution reactions are slow and poorly known. In contrast, at temperatures near 250°C rates of the same reactions will usually be fast enough to be ignored.

Wood and Walther (1983) have suggested that between 0 and 700°C silicates follow zero-order kinetics controlled by the surface area of reacting phases. Of more direct importance to the prediction of repository performance is the work of Moore and others (1983). These workers found that water passing through granite along a thermal gradient from 250-300°C to 80-100°C, reduced the permeability of the granite from 3 to 70 times. This reflected leaching of the rock at the higher temperatures, and the precipitation of silicate phases, closing off porosity at the lower temperatures. Similar work has apparently not been performed with tuff, salt or basalt.

Data is available on the solution rate of UO_2, the predominant component in spent fuel in oxidized solutions at low temperatures, (c.f. Grandstaff, 1976; and Amell and Langmuir, 1978), but not for reducing conditions or elevated temperatures. Wolery (1980) has estimated the effect of temperature on the dissolution rate of UO_2 for oxidizing conditions.

Adsorption and desorption reactions are generally complete in the range of seconds to minutes at 25°C unless they are diffusion controlled. Rates of such reactions are therefore fast enough to be ignored at higher temperatures. Rates of alteration of backfill materials such as bentonite above 100°C are poorly known, as is the nature of such alteration products.

Diffusion rates in the presence or absence of thermal gradients are poorly known for the radionuclides at low or high temperatures. Based on a literature survey, Apps and others (1982) assumed the diffusivities of radionuclides to be in the range from 1-5 x 10^{-10} m^2/sec. Based on such diffusivities, and assuming an unreactive backfill, significant concentrations of Pu were computed to escape through a 1 m backfill in less than 10 yrs, and through a 9 m backfill in less than 10,000 yrs. The reactivity of an actual backfill would greatly retard these diffusion rates.

Empirical ion diffusivities have been measured for Cs, Sr, and I in clay backfill and granite (Birgersson and Neretnieks, 1983). Skagius and Neretnieks (1982) measured effective diffusivities of 1-2 x 10^{-12} m^2/sec for Cs and Sr in granite, and 0.7 - 1.3 x 10^{-13} m^2/sec for iodide in granite. Rasmuson and Neretnieks (1983) suggest that this unexpected result may reflect migration of the Cs and Sr by both pore diffusion and by transport of the sorbed ions along intrapore spaces. However, the empirical data to establish the actual transport mechanism(s) is lacking.

On theoretical grounds ionic diffusivities can be expected to increase rapidly with temperature, however little or no data is available above 100°C for major ions, and none for uranium or the transuranics. Limited empirical data (Skagius and Neretnieks, 1983) show a reduction in the diffusivity of iodide with an increase in hydrostatic pressure (a 60% reduction for about

235 bars). In summary, not only are the diffusivities of radionuclides under repository conditions largely unknown, a theoretical basis for their prediction is also lacking.

Transport of solutes along a thermal gradient (Soret effect) is thought by some to be an important potential transport mechanism for radionuclides, particularly through the clay backfill materials surrounding the canister. Thornton and Seyfried (1983) measured the Soret effect between 300 and 100°C, at 600 bars over a distance of 30 cm in marine pelagic clay saturated with sea water. Major thermal diffusion effects were observed within 100 hrs with respect to Na, K, Mg, Ca, Cl, pH and ionic strength. The most important observation is perhaps not that enhanced ion transport occurred, but that water-rock reactions led to a reduction in clay permeability. This was caused by clay and anhydrite precipitation at the lower temperature. Soret effects will in any case be less significant at the lower anticipated temperatures (below 250°C) and for the greater thickness of clay backfill expected in a repository than used in the experiments of Thornton and Seyfried.

Osmotic effects (thermal osmosis and chemical osmosis) may also be important controls on radionuclide transport through clay backfill materials. Only theoretically predicted osmotic effects are available for repository conditions. Apps and others (1982) point out that such effects may lead to hydraulic gradients either towards or away from a canister, depending on the salinity difference between waters in the backfill and in surrounding country rock, and on the thermal gradient.

In summary, a variety of rate phenomena and irreversible processes will influence the mobility of radionuclides released from a repository. Probably the most important of these is the likely clogging of porosity and resultant reduction in permeability caused by solution of backfill or rock near the canister and the precipitation of secondary minerals in fractures and pore spaces at lower temperatures away from the canister. However, this phenomenon has not been studied experimentally in rocks other than granite. The results of the interplay of rate phenomena and irreversible processes under repository conditions cannot now be confidently predicted. Experimental studies are needed both to understand individual kinetic processes and irreversible reactions, and to examine the net effects of such reactions and processes for conditions expected in a repository environment.

4. Characterization of Background Conditions

It is essential that natural background conditions be established before repository construction and waste disposal. Such information is needed so as to allow prediction of the consequences of disposal, including proof after the fact of whether or not the biosphere has been contaminated. Accurate characterization of background conditions at repository depths demands the collection and analysis of ground waters and rock samples without their alteration or contamination by the sampling process. Ground water contamination by drilling mud is also likely when drilling in rocks of low porosity and permeability such as granites (c.f. Landstrom and others, 1983). With adequate care, such problems can apparently be avoided. Thus, three flowing subsurface boreholes drilled into granite in the Stripa Mine were evidently sampled without significant contamination (Fritz and others, 1979).

According to Hubbard (1984) contamination by drilling is not significant in the case of ground waters sampled from the Wolfcamp Formation and granite wash facies in the Palo Duro Basin of Texas. These sediments underly salt beds being considered as a repository. The relatively high porosity and permeability of the Wolfcamp and granite wash have produced sufficient ground water pumping rates to permit thorough flushing of any drilling mud prior to ground water sampling. Hubbard (1984) recommends downhole sampling for gases, but not for trace elements, which he has found to be lost by adsorption onto sampler walls.

The determination of in situ ground water pH and Eh conditions remains a problem. In most cases such conditions can be better computed than measured. Thus for deep boreholes the temperature, CO_2 pressure, and alkalinity can be used to compute the pH, as can temperature and CO_2 data, and the assumption (if reasonable) of calcite saturation. Eh calculation is best derived from information on the relative concentrations of electroactive species in the ground water, such as H_2S and native sulfur, or Fe^{2+} and suspended ferric oxyhydroxides, and the presence of minerals such as pyrite, ferric oxyhydroxides or siderite (see Thorstenson, 1970; and Lindberg and Runnells, 1984).

Recent studies by Krishnaswami and others (1983), and Laul and others (1983) have shown that analyses of the activities of naturally occurring daughter products of U, Th and Ra in ground water allows one to understand the geochemical behavior of these nuclides. Based on activity ratios of parent and daughter products one can infer, for example, that adsorption controls the dissolved concentration of the nuclide in question, and can compute the kinetics of the adsorption-desorption reaction. Such studies help one to predict the fate of nuclides of the same elements that might be released from a repository into the same water-rock environment.

Equally valuable is information on radionuclide mineral saturation state that can be computed from a ground water analysis using solution-mineral equilibria computer codes such as WATEQ described below. Such computations, based on analyses of ground waters in Swedish granites (Landstrom and others, 1983), and using an ion-interaction code for brines from the Palo Durq Basin of Texas, indicate that in both cases natural concentrations of U and Th are limited by the solubilities of UO_2 and ThO_2 of intermediate crystallinity. This suggests that precipitation rather than adsorption will limit maximum concentrations of U and Th isotopes released from a repository into the country rock. The calculation also indicates what the maximum concentrations of these elements will be (Langmuir, 1984). The shorter-lived nuclides of U and Th will be affected by solution-precipitation reactions in proportion to their relative concentrations compared to those of the long-lived isotopes. This assumes that rates of solution and precipitation are fast compared to the isotope half lives.

Also essential to the background characterization effort is age-dating of the ground water. Ground waters that contain tritium or C-14 are either surface contaminated, or so young (less than about 50,000 yrs) that the associated geological formation should not be considered for a repository. U-234/U-238 dating can sometimes give a useful relative age, but it is often of limited use because of unknown sources or sinks of uranium, especially in anaerobic water-rock systems. More useful for ground water dating are Cl-36 (half life 3.01×10^5 y) (see Phillips and others, 1983), and radiogenic isotopes of He, Ne and Ar (Hubbard, 1984). The use of Cl-36 is most applicable to fresh ground waters. In the high chloride brines associated with salt beds and salt domes Cl-36 is produced from Cl-35 by neutron activation at depth, thus reducing the sensitivity of the dating method. Hubbard (1984) prefers dating saline ground waters with the radiogenic isotopes of He, Ne and Ar, which he suggests indicate an age of about 130 my (between 60 and 260 my) for brines in the Wolfcamp Formation in the Palo Duro Basin of Texas.

Stable isotope data (especially oxygen and deuterium-hydrogen) for ground waters, fluid inclusions, and fracture and pore filling minerals such as clays and carbonates, provides uniquely valuable information regarding past and present sources of the ground water, whether meteoric or otherwise. Such data should be obtained along with a detailed petrographic study of the paragenesis of secondary mineral phases in the rock. Solution-mineral equilibria calculations for the ground water should yield mineral saturation results consistent with the presence of minerals shown petrographically to be of modern or youngest origin.

The concentrations and nature of occurrence of, for example U, Th and Ra in the country rock is also of considerable importance if we are to predict the fate of additional concentrations of these elements released from a repository breach. Are these elements present in the rock as discrete minerals, or in solid solution in carbonate, silicate, oxide or sulfate minerals for example? If so, what are the thermodynamic and kinetic properties of these phases in contact with the ground water?

5. Computer Simulation of Ground Water-Rock Reaction Chemistry

Computer models that allow calculation of the status of ground water-rock reaction chemistry have numerous applications to problems of high level nuclear waste disposal in geological formations. In most cases such models assume thermodynamic equilibrium, although a few such models include simple kinetic functions, such as those dealing with radioactive decay (see Pearson, 1983). Pearson (1983) adequately summarizes the characteristics of the diffferent types of models. Our discussion will be limited to model features, capabilities and limitations not covered in his narrative.

The two basic model types are static reaction state and mass transfer models (see Nordstrom and others, 1979). The static models [e.g. WATEQ series (Plummer and others, 1976), and SOLMNEQ (Kharaka and Barnes, 1973)] calculate the instantaneous thermodynamic condition of the water. Specifically, with input ground water chemical analysis, they calculate the thermodynamic activities of dissolved species and the degree of saturation of the water with respect to minerals. Complexation, redox, acid-base and gas-solution equilibria are also evaluated in the calculations. Kinetics and ground water flow are not considered. The second group of models, the mass transfer models, can calculate the amounts of mineral phases that must be dissolved or precipitated or species adsorbed to explain the observed changes in ground water composition between points along a ground water flow path [e.g. PHREEQE (Parkhurst and others, 1980) and EQ6 (Wolery, 1979)]. Some such models can also incorporate kinetic terms (EQ3/EQ6, Wolery, 1983)

Some of the static and mass transfer codes have been enlarged to include a thermodynamic data base for radionuclides including U, Th and Ra. Both model types have until recently been limited in their application to dilute ground waters (ionic strengths below about 0.1 m). This makes them useful for studies of most ground waters in tuff, basalt and granite, but not in salt. These models may be called ion pairing models. They employ Debye-Huckel or Davies equations to correct for the effect of ionic strength on ion activity coefficients.

Since about 1980, the ion-interaction approach to electrolyte solutions developed by Pitzer and his coworkers has been applied to the modeling of natural water-rock reaction chemistry in brines (c.f. Harvie and Weare, 1980). The model can accurately determine the mineral saturation state of brines with respect to major evaporite minerals including carbonates, but until recently had not been extended to the modeling of actinide geochemistry in brines. Since about 1982 the ion-interaction approach has been successfully used to model Ra and Sr (and Ba) reaction chemistry of brines (Langmuir and others, 1983, 1984). Ongoing research will add Th and U(IV) reaction chemistry to the model.

Adsorption modeling and its transport coupling in radionuclide studies has been largely restricted to the K_d approach. (A computerized data bank of radionuclide K_d values collected from worldwide sources is being assembled at the Nuclear Energy Agency in Paris.) However, the K_d approach cannot adequately account for expected variations in such adsorption-controlling properties of a water-rock system as pH, redox conditions, ionic strength, complexation, competitive adsorption, temperature, and variations in changes in the surface properties of sorbing phases (see Muller and others, 1983). Radionuclides are generally present in ground waters at trace concentration levels, under which conditions they tend to be adsorbed specifically, that is, against the net surface charge of sorbing minerals. A model which can incorporate all the variables that control and explain specific adsorption of radionuclides is the surface complexation ionization (SCI) model, introduced by Davis and others (1978). This model has been successfully used to explain the adsorption of U, Th, Ra and Pb by ferric oxyhydroxides (U), quartz and kaolinite (Th, Ra), and birnessite (Pb) (see Catts and Langmuir, 1983; Hsi and Langmuir, 1980, 1983, 1984; Hsi and others, 1982; Langmuir and Riese, 1982; and Riese and Langmuir, 1981, 1983). Cs adsorption by montmorillonite has similarly been modeled by R. J. Silva and others (1979). The SCI model is embodied in the computer program MINEQL (Westall and others, 1976), which has recently been combined with a transport code by Thomas Theis (Univ. of Notre Dame). A modification of the SCI model is presently being worked on to predict and explain radionuclide adsorption behavior in brines and at elevated temperatures.

6. Coupling Among Chemical, Hydrological, Thermal and Mechanical Effects

An excellent statement of the present capabilities and limitations of coupled modeling of effects is offered by Pearson (1983). The need to understand CHTM coupled effects obviously increases with an increase in the temperature of the waste canister and the magnitude and steepness of the thermal gradient from the canister to the country rock. One CHTM coupled process is backfill and rock dissolution near the waste with precipitation away from the waste at lower temperatures, which is likely in granite, and may also occur in some basalts, but not in tuff in the unsaturated zone. A second CHTM coupled process is the precipitation of minerals such as anhydrite and calcite around or on the canister because of their retrograde solubility with temperature. This effect is most likely in salt repositories where these minerals are already near saturation in most ground waters. A third CHTM effect is the possible change in clay backfill hydrological properties because of changes in, for example, the Na/Ca ratio with clay swelling at high Na concentrations. A fourth possible coupled effect is the thermal alteration of clay backfill materials, thus changing their HTM properties. In addition, thermohydrochemically coupled effects such as thermal diffusion, thermal osmosis, chemical osmosis, and ultrafiltration may occur. As pointed out by Pearson (1983), available computer models cannot accurately quantify effects such as described above. For this reason, the only answer at present is to design and perform complex laboratory and in situ field tests that closely simulate the conditions expected in a repository setting.

7. Implications for the Engineered Design of Backfills

The use of a bentonite clay backfill has been recommended for several reasons: first, because of the swelling properties of the clay and its low permeability, and second because of the high adsorption capacity of the bentonite for purposes of retarding radionuclide leakage.

A potential problem with such a backfill is the instability of bentonite at temperatures above 100°C, and especially at 250°C. A number of zeolite minerals are stable at the higher temperature, and have similar or higher adsorption capacities for radionuclides (e.g. analcime, chabazite, heulandite, stilbite and wairakite). These phases would be better choices than bentonite for adsorption purposes.

Another additive of value would be sulfidized ilmenite. Reaction of H_2S with ilmenite produces pyrite, which would poise the Eh of the backfill at low values and so minimize the oxidation of UO_2 and mobilization of uranyl species. The second product of sulfidization is amorphous TiO_2, which is among the most sorbent phases known for metal ions, including radionuclide cations.

Other possible approaches utilizing backfill, are to saturate the backfill with a water of higher salinity than the ground water in the country rock so that osmotic pressure effects would favor ground water flow towards the canister, not away from it. This same water could be pre-saturated with anhydrite and calcite to encourage canister armoring with these phases, thus inhibiting corrosion.

If the backfill were mixed with, say 5% uraninite ore, this could reduce the driving force for transport of uranium away from the canister.

Mixing in amorphous silica with backfill material would enhance the possibility of clogging the backfill and adjacent country rock by silica precipitation at lower temperatures, thus lowering permeabilities.

8. An Approach to Computer Simulation of Coupled Chemical Processes

As mentioned above (section 5), computer modeling will be required to assess many coupled processes, particularly those involving temperature, chemistry, and hydrology. Ideally, the temperature-dependent chemical, kinetic, and physical properties of all the possible phases that might be present over the span of time that a repository is to be effective should be incorporated into a transport code. The code should also handle double porosity media, changing physical and mechanical properties of the rock with changing temperature and changing mineralogy, two-phase fluid flow, and solutions of widely ranging compositions and salinities. Even if all the required data were available to put into such a code, it is unlikely that any presently available computer could handle the program. From a practical point of view, it is necessary that we look at restricted parts of the coupled systems, using enough variables to obtain significant results, but few enough variables to process in reasonable times with present computers. This would allow sensitivity tests to be made to determine what factors are likely to be important in more complicated models and what factors can be ignored. Some of these relatively simple systems should be investigated experimentally in the laboratory to verify the ability of the codes to predict what is observed. A second part of the verification process should be the application of computer codes to model the evolution of well-studied natural analog systems. If the "simplified" codes can successfully predict the formation and/or redistribution of the phases that actually filled fractures and changed the permeability, there is little reason to use more complicated codes that incorporate data for phases that are unimportant to the coupled process. Once the coupled T-C-H effects are in hand, the next step is to assume the time-dependent temperature and permeability distribution results obtained in the above model(s) and then incorporate that information within the computer models that deal mainly with rock mechanics, or with the transport of trace elements, including radioactive materials that might be released from canisters.

Equations of state for realistic compositions of repository fluids must be available in order to model coupled T-C-H processes. This is a trivial problem if temperatures remain below about 200 - 250°C. At progressively higher temperatures this becomes a significant problem, especially if appreciable dissolved gas is present. As a first (and probably good) approximation an equation of state for the system NaCl - H_2O can be used. The main concern is that the computer transport codes be based on the properties of saline solutions, rather than pure water.

Given the availability of appropriate computer codes that can model transport of boiling saline fluids through double-porosity rocks, the next step is to investigate the solution, transport, and deposition of various individual minerals. This requires knowledge of equilibrium solubilities and the kinetics of reactions as functions of temperature, salinity (ionic strength), pH, and, possibly, fugacities of oxygen and carbon dioxide. Minerals that should be modeled individually first and then in combination include quartz (and its polymorphs), calcite (and aragonite), and iron oxides. Computer codes and thermochemical plus kinetic information are currently available to model the behavior of quartz in dilute, hydrothermal solutions. Laboratory experiments are needed to verify the results of the computer simulations. In order to make T-C-H computer models applicable to real systems, feldspars and one or more ferromagnesian minerals must also be included as starting phases. This immediately requires that provision be made to account for the possible formation of solid solutions of many different hydrothermal alteration products, including clays, micas, and epidote.

9. Natural Analogs of Coupled Chemical Systems

Much attention is now being devoted to characterizing initial geologic, mineralogic, hydrologic, and rock stress conditions that are likely to be present within the various types of suggested repositories. This work is valuable and necessary to determine initial and boundary conditions. Less attention has been given to studies of analog natural hydrothermal systems that are presently at temperatures similar to those that are expected in repositories. These studies can provide information about (1) the minerals that are likely to form as hydrothermal alteration products, and their thermal and chemical stabilities, (2) the chemical and isotopic properties of the solutions, (3) the rates of movement of fluid through the systems, (4) the "instantaneous" distribution of thermal energy (temperature) in advecting and convecting situations, (5) the type, amount, and distribution of vein fillings, and (6) redistributions of the kinds of trace elements that are expected to be in the waste canisters. An excellent review of hydrothermal alteration studies that have been carried out in many kinds of rocks is given by Browne (1978).

Many studies of alteration in active hydrothermal systems in basalt in Iceland have been published (Kristmannsdottir, 1976; Kristmannsdottir and Tomasson, 1976a, 1976b). In the United States there are numerous hot-spring systems in basalt in Washington, Oregon, and Idaho that could be studied.

There are many published studies of "fossil" hydrothermal alteration related to ore deposition in granitic rocks. The solutions that were responsible for much of this alteration probably were much more acid than those that are likely to be present in a waste repository. There are few studies of alteration of granitic rocks in presently active hydrothermal systems because these kinds of rock have been less explored for geothermal resources. Hot-spring systems in granitic rocks have been drilled at Steamboat Springs, Nevada (Sigvaldason and White, 1961, 1962; Schoen and White, 1965, 1967) and at Coso, California (Hulen, 1978; Fournier and Thompson, 1980). A series of diamond cored holes at the margins of the Coso System are scheduled to be drilled by the California Energy Company. Low- to intermediate-temperature hot-spring systems that occur in granitic rocks could be investigated in Idaho, Montana and Colorado.

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DISCUSSION ON COUPLED FLUID DYNAMICS PROCESSES:

Coupled Processes of Potential Signficance

General Remarks

The most important mechanism through which radionuclides could be brought from a repository to the biosphere is the transport by groundwater. Such a process would start with the leaching of the waste, then the transport through the backfill and eventually through the rock formation to the surface. The leaching is by definition a coupled hydrochemical process, also coupled with thermal effects during the initial period when the waste is above ambient temperature.

Transport through the backfill (or any kind of engineered barrier) may be driven by pressure gradients, temperature gradients, osmotic effects or chemical gradients, or a combination of them. But the main concern about the backfill is its chemical or mechanical stability over long periods of time. Mechanical erosion cannot be ruled out in some circumstances, e.g. for clays (Push, 1983). Chemical transformation may increase the permeability (e.g. Na to Ca Bentonite transformation, Bentonite to Illite transformation), and such phenomena can occur in localized areas of the backfill (piping), breaching the barrier. Gas production from corrosion of the canister, or mostly from alpha-radiolysis by the waste, can perhaps breach the backfill by gas pressure buildup and fracturing. In salt, such gas production has been estimated to be on the order of a few m^3/yr per canister at a pressure of 9 MPa (Storck, 1984). This gas production can also play a role in the geosphere. Mechanical stability of the backfill can also be affected by seismic events (e.g. fracturing, compaction) or by the mechanical stability of the rock formation itself. Each of these mechanisms can enhance the transport of solutes towards the geosphere, thus being coupled with hydraulic effects.

Transport through the geosphere can take place either through the natural porosity of the rock, or through discontinuities in the rock resulting from the existence of the repository. Perhaps the major discontinuities are the tunnels and shafts themselves, and the disturbed rock immediately adjacent to them. Whether this disturbed zone and the repository backfill in the shaft and tunnels can play a major hydraulic role in transport of radionuclides through the geosphere depends upon the value of the permeability and porosity of these zones, compared to that of the undisturbed rock. It also depends upon the flow boundary conditions of the system, e.g. if a shaft or tunnel can be a short-circuit in the system between two more permeable zones of different hydraulic heads. Finally, the properties of the repository backfill may change with time, raising the same sort of question as the stability of the canister backfill.

Transport through the geosphere in the far field, away from the repository, is uncoupled only for nonreactive solutes. Any kind of interaction with the rock or other elements in solution makes it a coupled hydrochemical process.

In the following discussion a few items of concern for flow in the geosphere are outlined.

1. Thermohydrological Currents

For saturated media, the coupling T-H of the buoyancy effect is presently well understood and modelled in porous media; the uncertainty is (i) in the geometric description of the medium, especially for fractured systems, and also (ii) in the coupling with natural fluid pressure gradients and/or natural salinity and density variations in the media.

Methods of investigation are for (i) field studies, experiments and large scale testing, and for (ii) modelling studies.

It should be kept in mind that the thermally induced convective currents in a repository may bring to the waste containers ground waters of different geochemistry (e.g. salinity, redox potential) coming from deeper or shallower horizons. These waters may not have time to equilibrate chemically with the rock surrounding the canisters, and thus they may modify the geochemical near field in which corrosion and leaching occur.

For unsaturated media (e.g. tuffs), much less is known because of complex two-phase flow effects in porous-fractured media. Extensive laboratory studies, modelling and in situ testing are required. Among the principal uncertainties are phenomena relating to interference between the movements of liquid and gaseous phases, including (a) relative permeability, (b) capillary and adsorption effects, and (c) vapor pressure lowering. The mechanisms of gas phase transport (Darcy flow versus various diffusive mechanisms) need to be quantified for conditions applicable to the Yucca mountain tuffs. Also, some unusual mechanisms for liquid flow (chemical and thermal gradients) may be significant and should be studied. Many of the indicated effects may depend on temperature.

For salt, the potential influence of the convective currents induced by the heat load in the adjacent aquifers must be investigated along with salinity effects, especially by modelling studies. Thermally induced migration of fluid inclusions in the salt is presently under investigation.

2. Thermomechanical Effects on Fluid Flow

For fractured systems, very little is known about the quantitative prediction of the consequences of the thermally-induced stress field on the hydraulic conductivity of the system. The uncertainty lies in both the initial closing of joints during heating and the later reopening of the joints during cooling, because they may not return to their initial condition. Uncertainties are present both at the single fracture level (e.g. validity of the cubic law for large stresses) and at the network of fractures level. Both laboratory studies and large scale in situ experiments are required, because field studies under the appropriate stress levels cannot be duplicated in the laboratory. Thus, to investigate the thermomechanical effects, one must use the underground rock mass as the laboratory and keep in mind that the scale of the experiment must be large enough (tens to hundreds of meters) to realistically reproduce the repository conditions. No small-scale laboratory experiment can achieve this.

The possibility of the creation of new pathways is particularly important, e.g. by hydraulic fracturing because of pressure buildup if the permeability has dropped, or fracture openings caused by the development of tension stresses, or by piping effects (see also thermochemical effects). For salt, the problem of pathway creation should be investigated.

3. Thermochemical effects

The problem here is the quantitative prediction of the effect on the flowpath of the precipitation/dissolution of minerals in the rock. For fractured systems, this concerns both the fracture walls and fracture filling (Ribstein, 1983). For other rock media, it is especially related to the porosity. The effects of concern are:

- total clogging by precipitation, with a possible subsequent hydraulic fracturing effect.
- partial clogging, generating a piping effect, i.e. narrow passages in the fracture (or porous) network, in which the fluid velocity is higher, and the number of sites for adsorption much smaller. Radionuclide migration to the biosphere due to the thermal (or natural) currents would thus be much faster. Localized corrosion of the canister, or localized transformation of backfill could also result from piping.
- clogging of the pores of the matrix adjacent to a fracture, thus making matrix diffusion ineffective as a mechanism for slowing down radionuclide migration.
- dissolution (chemical dissolution, or pressure solution) capable of having a similar piping effect.
- for tuffs, the two-phase counter current flow (heat pipe effect) will generate precipitation towards the canister, and dissolution by the vapor phase and/or the capillary-attracted liquid phase, with possible chemical reaction (e.g. acid formation in the presence of chloride). These effects need to be investigated in carefully designed in situ field projects.

Another domain of interest is the study of the natural rate of clogging of fractures. The various fracture fillings of a system can constitute a record of the past rate of fracturing of the formation.

4. Dispersion in Fractured Media (C-H coupling)

Dispersion in single fractures due to the interplay between parabolic velocity profiles and molecular diffusion is well understood (Taylor dispersion). Very little is known about dispersion in fracture networks. Large values of the dispersivity for fractured media are reported in the literature. This effect must be understood and quantified. For example, the degree of connectivity within a network of fractures must play a key role in controlling dispersivity. To study such phenomena requires that one work with realistic fracture systems in the field.

As dispersion is a measurement of the variability of the velocity in the medium, it is directly related to natural "piping" phenomena in the media. Such effects are well-known in hydrothermal systems in fractured volcanic rocks, where tracer tests often show very rapid migration of tracers between wells. For many radionuclides of relatively short half-lives the confining power of the geologic barrier is brought about by the assumed small fluid velocities in the system, so variation in velocity is of utmost importance. If, for instance, 10% of the water flux has a velocity 10 times higher than the average, the resulting consequence (doses) can be orders of magnitude larger.

Of concern also is the effectiveness of matrix diffusion in the walls of fractures as a mechanism for slowing down transport. Here, analog studies are the best method of investigation.

5. Colloid Transport

Colloids can be present in a repository due to leaching of the waste, corrosion of the canister, degradation of the backfill, natural colloids in the groundwater, and precipitation processes. Colloids can contain radionuclides if they result directly from the leaching process (e.g. waste hydroxide colloids), but also if radionuclides in solution are sorbed on existing colloids, or if radionuclides are involved in coprecipitation reactions. Colloids tend to be unstable at high temperatures, but stable at low temperatures (i.e. below 50°C, at some distance from the waste, or during the cooling phase).

Colloids may or may not be sorbed, precipitated or "filtrated" (filtered) by the medium, depending on their electrical charge, which is a function of pH and groundwater composition. Migration of radionuclides to the biosphere in a colloidal (or complex) nonsorbing phase has been of concern for some time (Avogadro and de Marsily, 1983).

Very little is known of colloid behavior in fractures. The "hydrodynamic chromatography" effect must be high (i.e. velocities of small particles up to 1.4 times the average water velocity). Filtration must be present but less important than in porous media. Aggregation, precipitation and clogging must also be studied. Experiments are required both at the single fracture and the fracture network level.

In tuffs, very little is known of the behavior of colloids in the unsaturated zone, although the role of colloids in soil formation is quite important. Experimental studies should be initiated.

6. Aerosol formation

In the vicinity of a high-level waste package emplaced in unsaturated rock, vigorous boiling may occur which could eject small liquid droplets into the gas phase. An aerosol may form which can be transported along with the gas phase, and could carry liquid-soluble contaminants towards the biosphere. Laboratory experiments and theoretical studies should be undertaken to quantify this mechanism.

7. Gas Production

Chemical reactions (e.g. canister corrosion) and radiolysis can be a source of gas production in the medium. If the amount of gas production is large enough, a gas phase can develop, even in a saturated medium, when the solubility limit of the gas in the water is exceeded. In the safety study of waste disposal in salt at Gorleben, Federal Republic of Germany (F.R.G.), a figure on the order of a few m^3 of gas per year per canister at a pressure of 9 MPa has been estimated (Storck, 1984); the main source of this gas is in alpha-radiolysis by the waste. Such a gas production can create a fluid pressure buildup, if the medium is impervious. More likely, it can also create a two-phase flow system, where gas bubbles rise towards the surface, and in addition generate convective currrents in the liquid phase. Tests on these mechanisms are under way in the F.R.G.

8. Fracture geometry

Any fluid dynamic calculation in fractured media requires as a prerequisite an adequate understanding of the fracture network geometry. The present way of thinking is that the density and properties of the fractures themselves may dictate the approach that can be used for describing the medium:

- porous media equivalent for densely fractured media
- statistical description of the fracture network for low density fractures
- localization and description of each fracture for a very low density (sparsely fractured) network.

The development of mathematical models upon which prediction of long range effects rests so heavily must rely on the approach that is indicated at any given repository site. Recent work by Long and Witherspoon (1984) suggests that measurement of the density and average length may provide a way to build a dimensionless number that can be used to characterize the site. This points to the need for field work on this problem. The mapping that must be carried out requires access to an undergound test facility; otherwise the necessary details to describe the fractures cannot be obtained. Proof that the model is accurate will depend on certain in situ tests (hydraulic and tracer) being carried out in the same rock mass. This kind of combined theoretical and applied research should lead to methods of model validation that are crucial to other overall problems of site characterization.

Another fundamental need is to be able to generalize the fracture geometry as obtained from detailed measurements in the underground to the total rock mass through which migration is expected to take place. This means that the methods of geostatistics (Matheron, 1971; Delhomme, 1978; Journel and Huijbrecht, 1979; Beucher, 1983) must be investigated to detemine the field data that are needed to verify the spatial variability of the critical properties of the fracture network. The problem of extrapolating from the repository site to the flow system in the down gradient direction is the crucial issue. The applicability of geophysical techniques both between boreholes (e.g. tomography) and from the surface (e.g. sonic) to the underground also needs to be investigated as part of this overall problem.

9. Suggested Priorities for Fluid Dynamic Studies

Assuming the fracture system has been mapped in sufficient detail to provide a reliable model of the flow geometry, the following is a list of suggested priorities.

a. Large scale thermohydromechanical effects (see section 2)
b. Colloid transport (see section 5)
c. Thermochemical (precipitation/dissolution) (see section 3)
d. Thermohydrological currents (for tuff)
e. Dispersion effects (see section 4)

As a prerequisite we need a good understanding of the fracture geometry (see section 8).

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Table VI. Discussion on Coupled Fluid Dynamics Processes

1. Single Phase Flow and Transport (Saturated System - Far field)

   A. Single Fracture

      a - Effect of aperture, roughness and stress
      (tortuosity and connectivity for single fracture flow)

      b - Effect of deposition of material and infill material

      c, d - Effect of dissolution (pressure solution, chemical dissolution)

      e - Phenomena that control piping

      f - Diffusion into the matrix

      g - Taylor dispersion

   B. Network of Fractures

      a - Geometric description and distribution

      b - Effect of deformation (thermal, mechanical)

      c - Deposition/dissolution in network

      d - Buoyancy flow coupled with natural flow

      e - Dispersion, tortuosity, connectivity

2. Two Phase Flow and Transport (Coupled Fluid and Heat Flow)

   A. Tuff (Fractured - porous media)

      a - See 1B

      b - Relative permeability effects

      - capillarity and adsorption

      c - Gas diffusion (Binary, Knudsen, Thermal, Coupled)

      d - Counter-current two-phase flow, heat pipe effect

Table VI (continued)

e - Permeability changes due to phase change

- dissolution by vapor and condensate
- deposition from liquid and from vapor
- enhancement of chemical concentration and effects thereof
- fluid flow driven by concentration gradients
- change in thermophysical parameters (density, viscosity, vapor pressure)

f - Thermal osmosis

g - Advection, dispersion, and dead-end pore diffusion

B. Repository resaturation ("near-field")

a - Relative permeability effects

b - Dissolution of air

c - Leakage of air (pathway formation)

d - Capillarity and adsorption

3. <u>Particle Transport (colloids)</u>

A. <u>Single Fracture</u>

a - Hydrodynamic chromatography in fractures

b - Filtration in fractures

c - Clogging of fractures

d - Colloid aggregation and precipitation

B. <u>Network of Fractures</u>

a - Transport and filtration

C. <u>Tuff</u>

a - Filtration of colloids in the unsaturated zone

b - Aerosol formation and transport

Table VI **Coupled Fluid Dynamics Processes**

Dynamics of Fluid	Coupling	Potential Significance	Probability of Occurrence	Importance	Uncertainty Of Knowledge	Proposed Investigation Methods
1. Single Phase Flow and Transport						
A. Single Fracture						
a. Aperture, roughness, stress	5-HM	H	H	H	M	Lab measurements, large samples
b. Deposition of material	4-HC	H	H	H	H	idem
c. Dissolution (chemical)	4-HC	H	H	H	H	idem
d. Dissolution (pressure solution)	10-MCH	H	H	H	H	idem
e. Piping	11-TMCH	H	H	H	H	idem
f. Diffusion into matrix	4-HC	H	H	H	M	Analog studies and lab measurements on analysis
B. Network of Fractures						
a. Geometric description	none	H	H	H	H	Field investigation, large scale experiments
b. Deformation	8-HTM	H	H	H	M	Large scale experiment
c. Deposition-dissolution, piping	7-HCT	H	H	H	H	Analog - Large scale long term experiments
d. Buoyancy flow coupled with natural flow	2-TH	H	H	H	H	Modeling - Field experiments
e. Dispersion in network	4-HC	M	H	M	H	Modeling - Field experiments
2. Two-phase Flow & Transport						
A. Tuff (fractured-porous media)						
a. Behavior network f.p.m., see 1B	all	H	H	H	H	Modeling - Field Exp. Analogs - Large Scale Exp
b. Relative permeability effects	2-TH	H	H	H	H	Lab studies - modeling
c. Gas diffusion (binary, Knudsen, thermal, coupled)	7-TCH	H	H	H	H	idem
d. Counter current 2-phase flow	2-TH	H	H	H	H	Modeling - In situ experiment
e. Permeab. change due to mineral redistribution	7-TCH	H	H	H	H	Lab Studies - In situ experiment
f. Thermal osmosis	1-TC	H	H	H	H	idem
g. Advection, dispersion, pore diffusion	4-HC	H	H	H	M	Modeling - lab studies
h. Capillary & adsorption effects						
i. Fluid flow driven by chemical concentration gradients		M	M	M	M	Lab Studies - Modeling
j. Concentration-dependent changes in thermodynamic properties						

Table VII (continued)

Dynamics of Fluid	Coupling	Potential Significance	Probability of Occurrence	Importance	Uncertainty of Knowledge	Proposed Investigation Methods
B. Repository Resaturation						
a. Relative permeability effect	2-TH	M	H	M	M	In situ tests - Modeling
b. Leakage of air pathways	5-HM	H	H	H	H	idem
c. Dissolution of air	4-CH	L	H	M	M	idem
d. Capillary & adsorption effects						
3. Particle Transport (colloids)						
A. Single Fracture						
a. Hydrodynamic chromatography in fractures	4-HC	H	H	H	H	Lab studies - modeling
b. Filtration in fractures	4-HC	H	H	H	M	idem
c. Clogging of fractures	4-HC	H	H	H	H	idem
d. Colloid aggregation & precipit.	4-HC	H	H	H	H	idem
B. Network of Fractures						
a. Colloid transport in fractures	4-HC	H	H	H	H	In situ test - modeling
C. Tuff						
a. Colloid transport in unsaturated zone	4-HC	H	H	H	H	Lab studies - modeling - in situ tests
b. Aerosol formation and transport						

DISCUSSION ON COUPLED MECHANICAL PROCESSES:

Opening and Closing of Existing Fractures and Development of New Fractures

General remarks

Changes in the apertures of preexisting cracks in the host rock are likely to occur during the service life of a nuclear repository. These movements may influence the degree of containment if they result in an increase in the overall hydraulic conductivity. Changes in the opening of fractures are particularly important for those rock types in which water percolation takes place primarily through fracture networks, i.e. in hard rocks and to some extent in tuff. As the conductivity in such rocks is highly sensitive to the change in aperture of existing fractures and to the generation of new fractures, a detailed analysis of the underlying processes is recommended.

The discussion below follows the Outline of Coupled Mechanical Processes listed in Table VIII.

A. On "Opening and Closing of Existing Fractures":

1. Excavation of a Repository

A repository typically consists of a main shaft and a system of tunnels. Their excavation inevitably causes a redistribution of the initial state of stress in the surrounding rock, which in turn leads to deformations. Basically, two major phenomena may occur in an interactive way: deformation of the intact rock blocks bounded by discontinuities, and displacements of the blocks as a whole, resulting in opening and/or closing of the existing cracks. The extent of the change in the aperture depends on such factors as:

- o joint spacing, direction and persistency
- o deformability of intact rock
- o stiffness of joints
- o initial state of stress
- o size of the openings
- o method of excavation (smooth blasting, mechanical excavation).

Table VIII <u>Outline of Coupled Mechanical Processes</u>

		Coupling
A.	<u>Opening and Closing of Existing Fractures</u>	
1.	Excavation of a Repository	5
2.	Swelling of Fracture Fillings	9, 5
3.	Thermal Expansion	3, 9, 11
4.	Piping	11, 10
5.	Solution and Precipitation in Fractures	10, 11
6.	Creep in Salt	3
7.	Movements due to Regional Seismicity	5
8.	Fluid Pressure Opening and Closing Fractures	5, 9
B.	<u>Fracture Initiation</u>	
1.	Excavation of a Repository	5
2.	Triggering of Latent Seismicity	5, 9
3.	Thermal Cracking	3, 9
4.	Thermal Spalling	3, 5, 9
5.	Hydraulic Fracturing and Hydromechanical Effects	5, 9
6.	Stress Corrosion	11

Theoretical investigations based on a continuum model show that peaks of radial extensional strains and circumferential compressive strains occur at the excavation walls. They decrease, however, with increasing distance from the opening. This finding indicates that in a jointed rock mass those fractures which run tangential or nearly tangential to the walls of a shaft or of a tunnel will be particularly prone to opening. Existing joints which run nearly parallel and nearly radial to the axis of these excavations will tend to close. Between these two extremes any intermediate pattern may occur. In tunnels with horizontal axes, block movements in the roof may be exascerbated by gravitational forces acting toward the opening. In tunnelling this process is referred to as "loosening". The best way to assess the extent of fracture opening and closing around an excavation in a given rock type and at a given depth using a specific method of excavation, is to perform direct field measurements in large scale tests. Such tests may include the measurement of changes in the propagation speed of seismic waves through the fracture zone, and relative displacements in the rock using multiple point borehole extensiometers.

Reference: Terzaghi, K.: Introduction to Tunnel Geology in R. V. Proctor and T. L. White: Rock Tunnelling with Steel Support, Youngstown, Ohio (1946 and 1968)

NAGRA, Investigations of the loosening around a tunnel in hardrock, Switzerland (Report in prepratation).

2. Swelling of Fracture Fillings

Filling is the material separating the adjacent rock walls of discontinuities, and commonly consists of calcite, chlorite, silt, fault gauge, breccia, clay, etc. Clay, having a grain size less than 0.002 mm, has the particular property of volume expansion due to adsorption of water. Among the different clay minerals, the members of the montmorillonite group exhibit the greatest swelling capacity. In soil mechanics it is known that swelling is strongly related to stress relief. The relationship between swelling capacity and the logarithm of the normal stress in a consolidation apparatus is linear. Two parameters are sufficient to define this relationship. These are the swelling pressure index (pressure which is measured at zero volume change) and the free swelling strain index (which is measured at unconfined swelling). If the fractures of the host rock contain clay minerals, stress relief due to excavation of the opening will occur and cause swelling. The prerequisite for this, however, is seepage of water from the rock to this area. On the whole, swelling has a sealing function. Swelling and consolidation are well understood processes under room temperature conditions. The question of the long term properties of clay at elevated temperatures (over 100°C) is, however, not so well understood.

References: Int. Soc. of Rock Mechanics, Committee on Laboratory Tests, Suggested Method for Determining Water Content, Porosity, Density, Absorption and Related Properties and Swelling and Slake-Durability Index Properties, Int. J. Rock Mech. Min. Sci. 16, 1979.

Kassiff, G., Sharon, A. B. (1971): Experimental relationship between swell pressure and suction, Geotechnique 21.

Komornik, A., David, D. (1969): Prediction of swelling pressure of clays. Proc. Am. Soc. Civil Eng. 95.

3. Thermal Expansion

Thermal expansion is the change in shape and volume of a system due to temperature change. The host rock will be subjected to an increase and a subsequent decrease of temperature during the service life of the repository. On scales much larger than the individual grain size only volume change seems to be relevant; differential thermal strains between crystals do occur and this leads to microcracking that may affect the intrinsic permeability and porosity of the intact rock. In the host rock, thermal expansion takes place under confined conditions. This means that if the expansion of a given rock block is hindered, thermal stresses will be induced. However for every thermally induced compressive stress in a confined body, a reduction must occur in compressive stress elsewhere to maintain equilibrium. Volumetric expansion of rock blocks may cause the closing of existing cracks and fractures, leading to a reduced overall conductivity of the system, but the corresponding reductions in compressive stress may cause other cracks and fractures to open elsewhere. The extent of these changes in joint apertures depends on the thermal expansion coefficient of the rock and on the compressibility of the fracture surfaces. During the cooling period the reverse process is expected to take place. The average thermal expansion coefficient for the common types of rock in the range of 20 - 100°C is about $10^{-5}/°C$. The change in edge length of a cube having the size of 1.0 x 1.0 x 1.0 m due to 100°C change in temperature amounts to 1.0 mm. How thermal expansion actually influences fracture opening and closing in a particular rock mass can only be reliably answered by means of a large scale heating test, although the changes can be estimated using thermomechanical models.

Reference: S. P. Clark (Editor) Handbook of Physical Constants, The Geological Society of America, Inc., 1966, p. 94.

4. Piping

Piping is a process by which the flow conduits for fluids in media containing discrete zones of permeability may be enlarged. The enlarged opening permits accelerated flow, which can lead to further growth of the conduit. Piping occurs by both selective chemical solution and physical erosion (eluviation) of the walls of the conduit. The process is a function of the velocity and chemical state of the fluid, and the physical strength and solubility of the wall material. Physical piping is a common cause of serious damage in poorly constructed or natural dams where erosion of fine-grained soil particles can produce collapse of the dam. Chemical piping plays an important role in the develpment of karst topography by selectively dissolving limestone along fractures. It also is observed in the development of hydrothermal ore deposits.

Piping is a complex combination of chemical, hydraulic, mechanical and (sometimes) thermal effects. Though piping seems unlikely to occur in a waste repository, careful review of the literature on this subject and investigation of possible piping in the vicinity of a repository will be needed.

5. Solution and Precipitation in Fractures

Solution and precipitation within fluid-bearing fractures is a coupled thermal, hydraulic, chemical and mechanical process that controls the evolution of the fluid flow through fractures. As individual fractures become clogged with precipitates, local hydrostatic pressure may build up, new paths may be formed, and flow velocities along other fractures may change. Solution and precipitation will be affected by thermal, pressure and chemical gradients. When properly designed, with backfill of appropriate composition, the repository may be able to seal itself by means of a "precipitation front" forming at some distance from the repository. If the fractures are effectively sealed, could unsafe fluid pressure form around the canister? High fluid pressure could cause renewed fracturing or dissolution of precipitated components. If radionuclides are precipitated with the major constituents, we should be confident that the constituents could not be redissolved from the precipitated state as conditions change with time. The first step to evaluating solution and precipitation phenomena is to define the geochemistry of the site, and particulary of the expected fluid phases, thoroughly. This process is common and reasonably well described, qualitatively, in the literature on ore deposits.

6. Creep in Salt

One of the principal advantages of salt as a rock in which to excavate a repository is the prospect that excavations in rock salt will close by creep and that the wastes will eventually be encapsulated entirely, so that there will be no way by which the wastes can be released to the environment. If encapsulation were to occur in a usefully short period of time, say less than 1000 years, the problem of proving the long term performance of waste packages and other engineered barriers would be alleviated. Existing laboratory and field data concerning the creep of rock salt do not cover the ranges of stresses, temperatures and times that are likely to be applicable to the closure of repository excavations by creep of rock salt, so that it is difficult to decide with confidence whether or not complete encapsulation will occur or how long it may take. However, the creep closure of rock salt around waste containers and repository excavations can be modified by changes in stress concentrations, which depend upon the geometry of the excavations, and temperature, which depends upon the age of the wastes and the density at which they are emplaced in a repository, and the nature of any backfilling of the excavation. Coupled mechanical and thermal models are needed to investigate the interaction between these factors to determine whether or not encapsulation may occur within a usefully short period of time and to determine key conditions for creep so that lengthy laboratory measurements of creep can be focussed on the most relevant conditions.

Reference: Handin, J. W., Russell, J. E., Carter, N. L., Transient Creep of Repository Rocks: Mechanistic Creep Laws for Rocksalt, Final Report ONWI/SUB/79-E512-00900.

7. Movements Due to Regional Seismicity

The absence of seismicity at a site does not necessarily exclude seismicity as a consideration in evaluating the performance of a repository. Although distant earthquakes are not likely to damage the excavations of a repository, major earthquakes are thought to have brought about extensive changes in groundwater levels and flows at distances of hundreds of kilometers from the focus of these earthquakes. Proximate to the focus of an earthquake—

changes in stress may account for the observed groundwater changes. At great distances it is difficult to imagine how such changes occur, although it is presumably a result of the passage of the seismic waves. To produce changes of the magnitudes that have been observed, the effect of the seismic waves may be that of triggering latent instabilities in strain or dilatation. The processes involved have not been defined clearly but include, presumably, coupled effects between rock stresses and groundwater pressures. These effects are likely to be more complicated than would be expected from the simple theory of effective stresses, so that again coupled mechanical and hydraulic processes are involved.

8. Fluid Pressure Opening and Closing Fractures

Fractures generally provide the main conduits for the transport of fluid and mass in dense, crystalline rock masses. The conductivity of these fractures can be a very sensitive function of their aperture and hence of the fluid pressure and deformability of the fracture, while the fluid pressure itself depends importantly on the conductivity. In other words, the fluid flow is coupled to the deformability of the medium in which it takes place (Noorishad and others, 1971), through the effective stress law and Darcy's law. Construction of a repository, placement of the waste and the sealing off of the repository each cause perturbations of the fluid pressure field at the boundaries of the excavations. The effects on the fluid flow and hence its transport potential may be dramatic at each stage as apertures vary. Therefore, it is crucial to address this phenomenon along the lines of current investigations (Ayatollahi and others, 1983) on coupled hydromechanical effects.

References: Noorishad, J., Finite-Element Analysis of Rock Mass Behavior under Coupled Action of Body Forces, Flow Forces, and External Loads, Ph.D. Thesis, University of California, Berkeley 1981.

Ayatollahi, M. J., Noorishad, J. and Witherspoon, P. A., Stress-Fluid Flow Analysis in Fractured Rock Masses, J. Eng. Mech., Div. ASCE, Vol. 1, pp. 1-13, 1983.

B. On "Fracture Initiation":

1. Excavation of a Repository

The excavation of shafts and tunnels not only causes existing fractures in the vicinity of the excavations to open but it may also initiate the development of new fractures. The fracture initiation may be triggered by the stress redistribution around the opening and by blasting effects. The last factor, of course, is non-existent in the case of the application of a full face boring machine. Depending on the initial state of stress, the tensile strength of the rock, and also on its brittleness, the extent and degree of fracturing will differ. It is felt that new fractures will only develop in the close vicinity of an opening, i.e. in a range less than half the width of any free face of the opening. The roof area of a tunnel is especially prone to fracture initiation due to the direction of the gravitational force acting toward the opening. The greatest effect of new fractures on the hydraulic conductivity of the rock mass may reside in the enhanced interconnections between existing fracture conduits.

The importance of the excavation of the repository both on opening and closure of existing fractures and on fracture initiation must be carefully assessed. If the transport of nuclides to the biosphere along cracks and fractures adjacent to the tunnels and the vertical shaft turns out to be unacceptable, then counter-measures have to be considered such as the artificial filling of cracks by grouting.

Reference: Jaeger, C., 1979, Rock Mechanics and Engineering, 2nd ed.,
Cambridge Univ. Press, 523 p.

2. Triggering of Latent Seismicity

Major structures, such as large dams and mines appear sometimes to have perturbed tectonic equilibrium sufficiently to trigger local earthquakes, including quite large earthquakes ($M>4$) in regions thought not to be seismically active prior to construction. In regions that have been tectonically active, such as Nevada and the Pacific Northwest, rocks may be in a virgin state of stress very near failure at present. Even small changes in this state of stress brought about by the construction of a repository, or the superposition on the virgin state of stress of thermally induced stresses and changes in water pressure, could trigger seismic events of any magnitude. Although mines and dams as structures have proved to be quite resilient to earthquakes, it is not clear what effect local seismicity may have had on the hydraulic conductivity of the rocks around the structures. If the seismic activity were to involve a new fracture in a major stratum with low permeability, the effect on groundwater flow may be quite adverse. Conceivably, even the reactivation of a preexisting fault may also change its hydraulic conductivity sufficiently to have a significant effect. Effects such as these have not been studied extensively nor are they well understood. The processes involved are coupled in several ways. Triggering of latent seismicity could result from the perturbation of the virgin stresses in the rock by the excavation itself, but more likely, by thermal stresses or changes in water pressure. Although the seismicity itself may not be hazardous, the resulting changes in hydraulic conductivity of the strata could change groundwater travel times significantly.

It may be quite difficult to decide how close to instability is the virgin state of stress at a specific site. In all probability, rock stresses throughout a site vary in magnitude and direction in response to heterogeneities in the rock, especially jointing. Some parts of joints or faults may be very nearly unstable against sliding whereas other parts may be quite stable. The magnitude and distribution of these regions of different stability presumably determine the magnitude and distribution of seismic events that will occur if the virgin state of stress is perturbed sufficiently. The stresses that perturb the rock are induced by excavation, changes in water pressure, and thermal expansion, and these induced stresses can be estimated by numerical calculation. In situ stress measurements can be used to obtain estimates of the virgin stresses in the rock at those points where the measurements are made. The induced stresses can be superposed on the virgin stresses to determine the resulting total stresses at these points. Whether or not these total stresses will produce instability depends upon the strength properties of the rock. In heterogeneous rock, especially near joints and faults these properties are not known precisely, so that it is difficult to predict instabilities that will be induced by the changes in the conditions of total stress.

An alternative approach is to perturb the rock by a known amount and to measure seismically whether such perturbations produce instabilities. Prior to excavation, the rock can be perturbed by known amounts through changes in pore water pressure brought about by pressurizing boreholes. The magnitude of changes in pore water pressure necessary to produce instabilities provide a direct measure of the effects of changing the virgin state of stress. Furthermore, injection experiments can be designed to test the stability of quite large volumes of rock. Injection experiments must, however, be used with circumspection lest they produce hydraulic fractures that might impair the ability of the site to contain wastes.

Reference: First International Symposium on Induced Seismicity, Engineering Geology, Vol. 110, 1976.

3. Thermal Cracking

The development of heat in the repository will cause a temperature field to develop in the host rock. The intact rock consisting of an aggregate of minerals with more or less pronounced anisotropy is, even on a small scale, a heterogeneous material. When subjected to changes in temperature, stresses will occur which may lead to cracks either along the grain boundaries or through the grains themselves. Cracking or fracturing due to thermal effects is enhanced by the gradient of the temperature field. The gradient of the temperature field is expected on a large scale to show a decrease with increasing distance from the opening. On the other hand, a temperature gradient in blocks of rock bounded by conductive fractures may also occur due to the heat carrying capacity of the circulating water. Thus it is possible for new cracks to occur parallel to the existing ones, and in any other direction depending on the local tensile strength of the material, the initial stress state, and the prevailing thermal gradient. What is the possible influence of thermal cracking on the overall hydraulic conductivity of the rock mass? On the one hand, some of the existing cracks may close but, on the other hand, other cracks may open and the interconnections between fractures may increase to some extent. All these effects largely depend on the operating conditions of the repository, i.e. on the maximum permitted temperature in the host rock and on the properties of that rock.

4. Thermal Spalling

Thermal spalling occurs as a result of high, thermally induced compressive stresses parallel to a free surface. These stresses are most severe in the case of thermal shock when the temperature of a surface is suddenly raised to a high value. It is a dynamic process in which new surfaces are subjected to thermal shock as they are exposed by spalling. Thermal spalling is most pronounced in hard, brittle rocks and requires temperatures of several hundreds of degrees Celsius. Such temperatures are unlikely to occur even on the walls of boreholes in which waste canisters are placed. However, thermally induced stresses can also enhance conventional stress concentrations on the walls of boreholes or tunnels. As the combined value of the thermal stress and that due to the stress concentration approach the uniaxial compressive strength of the rock, progressive degradation of the walls can be expected. Such degradation was predicted and observed in the experiments at Stripa.

Reference: Cook, N. G. W., Myer, L. R., "Thermomechanical Studies in Granite at Stripa, Sweden," Advances in the Science and Technology of the Management of High Level Nuclear Waste, Battelle, Ohio, 1981, ed. by P. L. Hofmann and J. Breslin.

5. Hydraulic Fracturing and Hydromechanical Effects

When water pressures in rock exceed the normal stress across any plane and the tensile strength of that plane, a hydraulic fracture is produced. In solid more or less isotropic rocks, the plane of a hydraulic fracture will tend to be oriented so that it is normal to the direction of the minimum compressive stress in the rock. In bedded and jointed rocks, the strength of these surfaces of discontinuity may be so low compared with the tensile strength of the rock that hydraulic fractures may propagate along, and open up, such weaknesses more easily than producing a new fracture. Surfaces of weakness in rock are not necessarily oriented so that they coincide with the directions of the current principal stresses, and shear stresses may exist across such surfaces. (In such cases, the reduction of normal stress across these surfaces by the pressure of the water may reduce frictional resistance to sliding by an amount sufficient to allow sliding motion between the surfaces.

Such motion may occur in an unstable manner as a seismic event. Seismic events have been discussed separately under section 2, Triggering of Latent Seismicity.) Opening of new or preexisting surfaces by hydraulic pressure will change the hydraulic conductivity of the rock. Hydraulic fracturing phenomena must, therefore, be considered in determining the performance of a repository.

Prior to excavation, hydraulic heads in the rock at a repository site are likely to be closer to hydrostatic values than to lithostatic values. Drainage into the repository excavations during construction and until some considerable time after closure of the excavations will have the effect of decreasing hydraulic pressures from their virgin values. The overall effect of diminishing hydraulic pressure is to stabilize the rock and to close any fractures or joints that may have existed originally. Some period after closure of the repository the residual voids will become filled with water. Should this occur while temperatures in the repository are still increasing, the pressure of the water will increase as a result of the high coefficient of thermal expansion for water ($4 \times 10^{-4}/°C$) compared with that for rock ($10^{-5}/°C$). If such an increase in volume is produced by thermal expansion, the pressure of this water will rise until it either produces a hydraulic fracture or opens preexisting surfaces of discontinuity of the rock assuming that the resaturated medium has become impermeable (e.g. by clogging due to precipitation); otherwise, the pressure buildup will cause the groundwater to flow (convective currents). The water pressure needed to do this must be greater than the value of the minimum principal stress in the rock.

Potential problems involving the possibility of hydraulic fracturing produced by thermal expansion should be considered and resolved during the design of any repository. It seems that if the peak of the temperature pulse occurs before the repository excavations become refilled with water, hydraulic fracturing may not become a problem. Even if this cannot be achieved, it should be possible to arrange the period of the refilling cycle, the period of the temperature pulse, and the volume of water in the repository excavations in relation to the properties of the surrounding rock and the state of stress in it, such that hydraulic fracturing poses no threat to the performance of the repository. Clearly, this evaluation involves consideration of thermal, mechanical and hydraulic effects.

Reference: Workshop on Hydraulic Fracturing, Menlo Park, 1981, ed. M. Zoback, and B. Haimson, National Research Council, Washington, D. C. 1982.

6. Stress Corrosion

Stress corrosion is the process of differential weakening of a rock at the tips of cracks due to chemical attack. This process is apparently responsible for both the creep of brittle rock and subcritical crack growth in the presence of a chemically active species, including liquid water or water vapor. Because the crack tip is a highly stressed location, corrosion takes place at an accelerated rate. The experimental measurement of the effect and the chemical explanation of the phenomenon are still the subject of a considerable amount of research (e.g. Costier and Mecholsky, 1983; Johnson, 1983; both in Proc. 24th Symp. Rock Mech., Texas A&M). In terms of repository design and performance, it has the effect of diminishing the tensile strength of the rock and hence accentuating cleavage fracture phenomena.

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5. Tables of Coupled Thermo-Mechanical-Hydro-Chemical Processes

Table 1: Thermochemical Processes

Table 2: Hydrothermal Processes

Table 3: Thermomechanical Processes

Table 4: Hydrochemical Processes

Table 5: Hydromechanical Processes

Table 6: Mechanical-Chemical Processes

Table 7: Thermohydrochemical Processes

Table 8: Thermomechanical-Chemical Processes

Table 9: Thermohydromechanical Processes

Table 10: Hydromechanical-Chemical Processes

Table 11: Thermohydromechanical-Chemical Processes

#1 T–C

THERMOCHEMICAL PROCESSES

Process	Significance	Uncertainty	Misc: Methods of Investigation, other comments
Speciation	H	H for Nuclides components L for major species components H for high temp. and press. H for kinetics	
Complexation	H		
Thermal Diffusion	H		
Phase Changes	H		
Equation of State (see #4 HC)	H		
Solid Solution	H		
Metastable Phases	H for low temp. (phase type dependent) H for high temp near Backfill		

#2 T–H

HYDROTHERMAL PROCESSES

Process	Significance	Uncertainty	Misc: Methods of Investigation, other comments
Convective Currents 1 or 2 phases	H	L*	Problem of path determination
Phase Change and Interference	H	H for Tuff in Near field and Far field H for other rock types in Near field	Problem of characterization of fractured porous media
Thermophysical Property Changes	H for Tuff	H for Tuff	
Thermal Osmosis	H for Tuff H for all in Backfill	H	
Gas Diffusion Binary Knudsen Thermal Coupled	H for Tuff	H for Tuff	Experiments
Capillary-Adsorption	H for Tuff	H	

* Question of modeling behavior assuming NaCl solutions.

#3 T ⇔ M THERMOMECHANICAL PROCESSES

Process	Significance	Uncertainty	Misc: Methods of Investigation, other comments
Induced Cracking	M	M	
Fracture Deformation	M	M	
Thermal Spalling	H for Near field	L	
Thermal Creep	H for Salt L for others	H	
Thermal Expansion Uplift or Subsidence	M	L	

#4 H = C HYDROCHEMICAL PROCESSES

Process	Significance	Uncertainty	Misc: Methods of Investigation, other comments
Solution	H	Temperature L 25°C H T>100°C Concentration L Dilute H Brines Phases L Gas phase at low temperature H Gas phase high temp.	
Deposition	H		
Sorption	H		
Desorption	H		
Redox Reactions	H		
Complexation	H		
Hydrolysis	H		
Acid-Base Reactions	H		
etc.			
Diffusion	H		
Chemical Osmosis	H	H in unsaturated rock	
Isotopic Exchange	H		
Co-precipitation	H		

#5 H=M

HYDROMECHANICAL PROCESSES

Process	Significance	Uncertainty	Misc: Methods of Investigation, other comments
Hydraulic Fracture	M	M	
Pore Pressure Change	H	L	
Mechanical Erosion of Fractures	M for water as the fluid	L	
Sedimentation of Particles	M	L	
Shear Effect Causing Abrasion	L	L	
Variation of Fracture Apertures	H	H	Experiments

#6 C—M

MECHANICAL-CHEMICAL PROCESSES

Process	Significance	Uncertainty	Misc: Methods of Investigation, other comments
These processes will be modified by water flow and the thermal field, so they should be incorporated into processes #7 THC and #8 TMC.			

#7 

THERMOHYDROCHEMICAL PROCESSES

Process	Significance	Uncertainty	Misc: Methods of Investigation, other comments
Solution/Precipitation	H for all rock types	L for Salt M for Basalt H for Granite	
Solution and Precipitation Kinetics	L for Salt* H for all others	L for Salt H for all others	Analog studies More modeling; most important at low temp
Fluid Transport by Osmotic Effect	H for Tuff H for Backfill Unknown for Salt	H for Tuff H for Backfill	Experiments
Chemical Transport in Gas Phase; Partition between Gas and Solid	H in Near field	H in Near field	Lab; Theory; importance of boiling
Particle Transport (Colloids)	H in Near field except L for Salt**	H for all	Lab; Dilute systems, low temp.
Equation of State	H	H for high temp.	
Thermal Diffusion (Soret Effect)	L except H for high temp. gradient		

*Minerals in salt deposits equilibrate with water rapidly.

**Colloids are unstable in saline waters.

#8

THERMOMECHANICAL-CHEMICAL PROCESSES

Process	Significance	Uncertainty	Misc: Methods of Investigation, other comments
Phase Change in Mineral Phases	L	M	
Dehydration	M for Near field and Backfill	L	
Creep	May be important for Salt and in Backfill		
Hydration and Swelling	H for Near field and Backfill	L	

Note: Could be included in #11, THMC

#9 

THERMOHYDROMECHANICAL PROCESSES

Process	Significance	Uncertainty	Misc: Methods of Investigation, other comments
Hydraulic Fracturing	H for impermeable brittle rock, with water	M	Calculation; Field experiment; analysis
Triggering of Latent Seismicity a. Stress Redistribution b. Pore Pressure	M	H	In-situ stress measurement; maybe prevented by careful screening
Opening and Closing of Joints a. Stress Redistribution b. Thermal Coupling c. Pore Pressure	H for all rock types except Salt	M	Field experiment; uncertainty in properties
Spalling	L	M	Could be under #8 TMC
Change of Strength Hydrolytic Weakening	M	M	
Hydration			Could be under #8 TMC

#10

HYDROMECHANICAL-CHEMICAL PROCESSES

Process	Significance	Uncertainty	Misc: Methods of Investigation, other comments
Isothermal Precipitation (clogging pores)	M for Far field	H for all rock types except Salt	
Stress Corrosion	M	M	

This category of coupled processes was eliminated from consideration because without the temperature gradient the mass transport is not sufficient to change the geometry, except for low temperature precipitation and pressure solution, $T \leq 50$ C.

#11 T ☒ H
M C

THERMOHYDROMECHANICAL-CHEMICAL PROCESSES

Process	Significance	Uncertainty	Misc: Methods of Investigation, other comments
Piping a. Selected Dissolution and Tunnel Corrosion b. Inhomogeneous Leaching	H for Salt and fracture fillings for hard rocks	H	Review of data in geothermal, dams, salt etc.; may interconnect repository to existing fractures
Precipitation a. in Fractures b. in Matrix	M	H	
Hydrothermal Alteration of Rock			
Heat Pipe Effect with Dissolution/Precipitation	H for Near field	H	
Vertical Vapor-Liquid Cycling near Canisters			
Pressure Solution	H for Near field	H	

6. CONCLUSION

The present report summarizes the discussions and findings of the first of three Panel meetings planned over FY 1984-86.

The scientific and technical problems associated with the optimal design of an underground nuclear waste repository are multidisciplinary. This report attempts to address processes which result from couplings among phenomena studied by different scientific disciplines, such as geohydrology, geomechanics, and geochemistry. Since we are interested in the long term performance of a repository over thousands of years or more, some coupled processes not normally expected to be significant over a 10 - 50 year period may become very important. Hopefully this report, with its tables, has identified most of these processes.

All of the tables and discussions presented here are preliminary in nature and will be modified and improved during the next two Panel meetings, based on comments from the scientific community and new research findings. Below we shall bring out a few initial observations of particular interest, which are not meant to summarize the report nor to be all-encompassing recommendations, but to draw attention to certain issues considered to be significant with our present knowledge. The readers are encouraged to review the whole report.

1. There are substantial reasons to limit the maximum temperature in the near field (and, of course, the far field) to below 250°C, and, if possible, below 100°C. There appears to be a particular lack of various hydrochemical data, especially in the range of 30 - 250°C.

In addition, solubility and other temperature dependent properties undergo a drastic change at approximately 250°C. So it is suggested that the maximum temperature be kept below 250°C. Furthermore, all chemical reactions (e.g. corrosion of the canister, transformation of the backfill, etc.) are considerably slowed down as temperature decreases, thus improving the safety of disposal. If the maximum temperature is limited to 100°C, the potential development of a vapor phase is also eliminated. In addition, because of the lack of an adequate data base of hydrochemical data, a lower limit is desirable since extropolations of data to 100°C may be done with more reliability than extropolations to higher temperatures.

2. One process that has not received much attention is the piping effect--i.e. the formation of fluid flow channels due to pressure solution, etc. Such effects are known in the fields of mining and soil mechanics. A review of the literature and some laboratory tests are needed to determine its significance in the design of a nuclear waste repository, initially in the canister and backfill, but also eventually in the host rock.
3. In media other than salt, most problems appear to revolve around the behavior of discontinuities in the rock, such as joints and fractures. The thermal, mechanical and hydraulic processes occurring in these features are not well understood, particularly when they are coupled.
4. A number of other processes deserve further attention, particularly steam-water counter flow and its coupling with chemical dissolution and deposition, if the maximum temperature limit is greater than 100°C. There are important unanswered questions of the significance

of a number of other processes, such as colloidal transport of radionuclides, gas production by radiolysis, seismicity triggered by thermomechanical loading, and permeability changes due to various chemical and mechanical processes.

5. There is a wealth of data on hydrothermal systems, especially in the areas of geochemistry and economic geology. A carefully planned and thorough study of natural analog systems would yield useful information for the design of a nuclear waste geological repository.
6. The need for laboratory and large-scale in situ testing to study and determine the significance of various coupled processes cannot be overemphasized, as it seems to be the only way in which some of these questions can be answered.

Summary

Four basic physical processes, thermal, hydrological, mechanical and chemical, are likely to occur in 11 different types of coupling during the service life of an undergound nuclear waste repository. A great number of coupled processes with various degrees of importance for geological repositories were identified and arranged into these 11 types. A qualitative description of these processes and a tentative evaluation of their significance and the degree of uncertainty in prediction is given. Suggestions for methods of investigation generally include, besides theoretical work, laboratory and large scale field testing. Great efforts of a multidisciplinary nature are needed to elucidate details of several coupled processes under different temperature conditions in different geological formations. It was suggested that by limiting the maximum temperature to 100°C in the backfill and in the host rock during the whole service life of the repository the uncertainties in prediction of long term repository behavior might be considerably reduced.