KBS TEKNISK RAPPORT

06

GROUNDWATER MOVEMENTS AROUND A REPOSITORY

Phase 1. State of the art and detailed study plan

Hagconsult in association with Acress
Consulting Services Ltd and RE/SPEC Inc.

77-02-28

Objekt 19.03

KÄRN - BRÄNSLE - SÄKERHET

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I slutet av rapporten har bifogats en förteckning över av KBS hittills publicerade tekniska rapporter i denna serie.

KBS-Kärnbränslesäkerhet

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FOREWORD

This report was prepared as the first phase of a study of the groundwater movements around a repository for spent nuclear fuel in the precambrian bedrock of Sweden. The contract for this work was between KBS-Kärnbränslesäkerhet (Project Fuel Safety) and Hagconsult AB of Stockholm, Sweden. RE/SPEC Inc. of Rapid City, SD/USA and Acres Consulting Services Ltd of Niagara Falls, Ontario/Canada acted as subconsultants to Hagconsult AB.

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The opinions and conclusions expressed in this document are those of the authors and should not be interpreted as necessarily representing the official policies or recommendations of KBS.

Stockholm, February 28, 1977

Ulf E. Lindblom
Study Director
Hagconsult AB

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1. INTRODUCTION

This report summarizes the conclusions and recommendations reached in the Phase 1 studies as outlined in the Hagconsult proposal entitled "Radioactive Waste Repository for Sweden - Long Term Containment Safety: Study based on rock mechanical, hydrogeological and thermal analyses", dated December 1976. The objectives of these studies are to provide a state of the art review of groundwater flow in the region of a repository in granitic rock, in order to provide a basis for long term containment assessments and to prepare a detailed study plan for the continuation of the project.

We present a general description of the problem, including a summary description of the spent fuel and expected site geology, together with a qualitative description of the expected response of the reference repository concept. In addition, the different processes affecting the groundwater situation for containment are given.

In section 3, we present a state of the art review of the fluid flow, geochemical, heat transfer and rock mechanics processes as they relate to containment. In each case, data availability, prediction and validation procedures and monitoring techniques are discussed.

In section 4, we present a detailed study plan to provide a comprehensive assessment of the hydrogeological regime around the repository during its lifetime. This necessarily requires treatment of many complex coupled processes and is based heavily on the use of mathematical simulation models which will be validated against available field test data. The groundwater flow fields will provide a basis for subsequent long term containment studies.

2. PROBLEM DEFINITION

2.1 Description of spent fuel

The composition by weight of the fuel in Swedish boiling water reactors is summarized in Table 2-1. Calculated activities of actinides and fission products in the spent fuel are summarized in Tables 2-2 and 2-3, respectively. All of these data were taken from the Swedish Aka report entitled "Spent Nuclear Fuel and Radioactive Waste" (1976).

It can be assumed that the fuel elements are stored about 15 years before emplacement in the repository. The heat generation rate at emplacement can be calculated as 200W per canister, and approximately 20W after 90 years of storage.

The conditioning of the fuel elements is not yet known. However, it might be assumed that they will be somehow encapsulated in glass or in super-resistant compounds fabricated by hydrostatic forming processes.

2.2 Geological description of proposed sites

The Fennoscandian shield of precambrian bedrock dates back more than 600 million years and is composed of the "roots" of very old eroded rock formations. Dominating rocks in the shield are those of the metamorphic type, e.g. gneisses, magmatic type, e.g. granites, and recrystallized surface rocks. In addition, there are sedimentary rocks, e.g. sandstones, shales and limestones consolidated to quartzites, and precambrian limestones, dolomites, shales and leptites, and volcanics, such as tuffs. These rocks exemplify the earth's oldest rock formations. There are many areas with these types of rocks on the earth's crust in spite of several periods of mountain formation.

Location of rock types such as tillites and conglomerates, which originate from till composed of a mixture of boulders, gravels and sands of precambrian age,

Table 2-1. Composition by weight of spent fuel

Element	Percentage by weight
Uranium - 235	0, 8
Uranium - 236	0, 3
Uranium - 238	95, 0
Fissionable plutonium	0, 6
Other plutonium	0, 3
Other transuranium	0, 07
Fissionproducts	2, 9

Table 2-2. Actnides in spent fuel

Nuclides		Curie per ton uranium in fuel after		
		30 days	180 days	2 years
Curium	-246	0, 06	0, 06	0, 06
	-245	0, 30	0, 30	0, 30
	-244	1700, 00	1700, 00	1600, 00
	-243	17, 00	16, 00	16, 00
	-242	34000, 00	18000, 00	1700, 00
Americum	-243	15, 00	15, 00	15, 00
	-242m	13, 00	13, 00	12, 00
	-241	140, 00	210, 00	470, 00
Plutonium	-242	1, 80	1, 80	1, 80
	-241	116000, 00	113000, 00	105000, 00
	-240	510, 00	510, 00	510, 00
	-239	300, 00	300, 00	300, 00
	-238	1700, 00	1800, 00	1900, 00
Neptunium	-239	1900, 00	15, 00	15, 00
	-238	26, 00	13, 00	12, 00
	-237	0, 21	0, 21	0, 21
Uranium	-238	0, 32	0, 32	0, 32
	-236	0, 22	0, 22	0, 22
	-235	0, 016	0, 016	0, 016
	-234	0, 74	0, 75	0, 75

Table 2-3 Fission products in spent fuel

			Curie per ton uranium in fuel after		
Nuclide		Half life	30 days	180 days	2 years
Tritium	-3	12, 33 years	700	690	640
Carbon	-14	5 730 years	0, 4	0, 4	0, 4
Krypton	-85	10, 73 years	8 800	8 600	7 800
Strontium	-89	50, 85 days	470 000	64 000	41
	-90	29 years	66 000	66 000	63 000
Yttrium	-90	64, 0 hrs	66 000	66 000	63 000
	-91	58, 6 days	630 000	110 000	160
Zirkonium	-93	950 000 years	1, 6	1, 6	1, 6
	-95	65, 5 days	840 000	170 000	480
Niobium	-93m	12 years	0, 1	0, 2	0, 3
	-95	35, 1 days	1 100 000	330 000	1 000
	-95m	3, 61 days	17 000	3 600	10
Teknetium	-99	213 000 years	12	12	12
Ruthenium	-103	39, 6 days	570 000	41 000	2, 7
	-106	1, 01 years	390 000	300 000	105 000
Radium	-103m	56 min	560 000	40 000	2, 6
	-106	29, 9 sec	390 000	300 000	105 000
Tin	-126	100 000 years	0, 48	0, 48	0, 48
Antimony	-125	2, 73 years	7 100	6 500	4 400
	-126	12, 4 days	69	0, 09	
	-126m	19, 0 min	0, 48	0, 48	0, 48
Tellurium	-125m	58 days	1 500	1 500	1 000
	-127	9, 4 hrs	7 100	2 600	80
	-127m	109 days	6 900	2 600	80
	-129	70 min	111 000	510	
	-129m	33, 4 days	17 000	800	
Iodine	-129	15, 9 mill.years	0, 025	0, 025	0, 025
	-131	8, 041 days	50 000	0, 012	
	-132	2, 285 hrs	1 700		
Xenon	-131m	11, 99 days	1 500	0, 031	
	-133	5, 29 days	32 000		
Cesium	-134	2, 06 years	120 000	110 000	64 000
	-135	2, 3 mill.years	0, 38	0, 38	0, 38
	-137	30, 1 years	94 000	93 000	90 000
Barium	-137m	2, 55 min	88 000	87 000	84 000
	-140	12, 79 days	240 000	71	
Lanthanum	-140	40, 23 hrs	280 000	82	
Cerium	-141	32, 53 days	600 000	26 000	0, 2
	-144	284, 4 days	830 000	570 000	150 000
Praseodynium	-143	13, 58 days	260 000	120	
	-144	17, 28 min	830 000	570 000	150 000
Neodynium	-147	10, 99 days	68 000	5, 9	
Promethium	-147	2, 62 years	120 000	110 000	71 000
Samarium	-151	93 years	440	440	430
Europium	-152	13 years	12	11	10
	-154	16 years	4 800	4 700	4 400
	-155	4, 8 years	2 100	2 000	1 600
	-156	15, 2 days	33 000	32	

reveal the existance of glacial and erosion periods already at this early time. Contrary to most places in the world, the Fennoscandian shield was cleaned and worn down by the latest glacial ice and is today covered by little or no surface soil.

During previous geological periods, the precambrian shield was subjected to different states of stress, so called tectonic disturbances, leading to a cracked and altered rock mass. Thus, the precambrian shield is traversed by failure planes, crushed and weathered zones, separating the rock mass into a pattern of zones of competent and unfractured rock. The lateral distance between these zones can vary from hundreds of meters to several kilometers, or to even tenths of kilometers. Along many of these failure zones, movements have occurred. Nature itself has often healed crushed zone products, developed during the shear motions; thus, grained as well as coarse crushed materials were regenerated into hard rocks (e.g. breccia). However, failure zones are often zones of weakness composed of low quality, fractured and altered rock material.

The rocks of the precambrian shield are crystalline, hard and practically water impermeable; i.e., any significant permeability in the crystal matrix will usually not exist. In spite of this, the rock mass is usually water bearing due to the existance of cracks and crushed zones. Construction in rock, in the form of mines, rock chambers and tunnels, drillholes for water and exploration, and blasting operations on the ground surface has provided a certain knowledge of the fractured and crushed zones of the bedrock. A rule of thumb for water drillholes in rock says that there exists a fractured water-bearing rock down to a depth of 30-40 meters, and that drilling should be discontinued if water is not found in the first 100 meters of depth. Large amounts of water can, however, be found at greater depths; but the drillhole would have to be directed such that it intersects a large crushed zone in the rock at great depth.

An impression of the degree of fracturing of the bedrock can usually be obtained from the surface rock which outcrops in road cuts and rock chambers and in tunnels and excavations in the upper portion of the crust. Between large failure zones in the shield along which so called block moments have occurred and are occurring, rock portions with low permeability may be found at a depth of 100 meters or more. Although the rock blocks have not been disturbed during millions of years, one cannot completely determine the existence of a network of fine cracks. The groundwater which has penetrated these fine cracks down to great depths, is judged to be isolated and very old. With the new technique of drilling tunnels with the so called full-face machines, a better method has been developed for studying the cracked and crushed zones of the precambrian shield without blasting damage. These studies have given further evidence that there exist at depth relatively large blocks of rock with very low frequency of cracks and that the width of these cracks is very small.

2.3 Reference repository concepts

Repository locations under consideration in Sweden are all located at great depth (at least 500 m) in the precambrian granitic bedrock.

In 1976, the Swedish government committee on radioactive waste (Aka, Sou 1976:31 p 118, 126), discussed a reference concept which in principle corresponded to a mine with shafts, tunnels and drillholes, to contain the waste. Backfilling was expected to take place after the operational life of the repository. The proportion between shafts, tunnels and drillholes was not fixed, but seen as possible to vary between wide limits. Asphalt and magnetite-bearing cat-ion adsorbing clay were suggested as sealants for the drillholes, cf. Figure 2-1. The waste was assumed to be solid glass, encapsulated by a resistant watertight mantle. A multiple containment was thus envisaged, where the low permeability of the surrounding crystalline rock, the low solubility of the glass and the encapsulation should give a threefold protection against the dispersion of the waste. It was suggested that additional protection could be achieved by surrounding each waste-cylinder by a layer of cat-ionretaining clay. Further the small volumes of groundwater passing the waste, its long residence time in the rock enhanced by processes of adsorption, were referred to as natural barriers against the active waste reaching the surface of the Earth.

A recent concept that has been proposed for a Swedish spent fuel repository is shown in Figure 2-2. A system of fairly large tunnels will be blasted in

1. Sand backfilling
2. Asphalt plug
3. Sealant ion exchange clay with magnetite
4. Resistant canister
5. Spent fuel
6. Granite bedrock

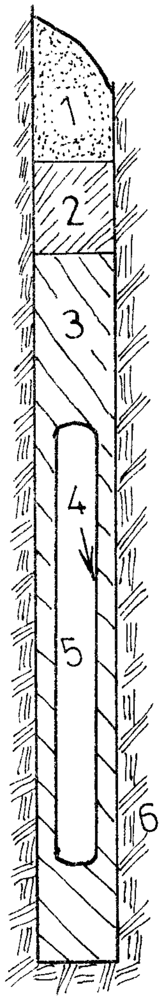
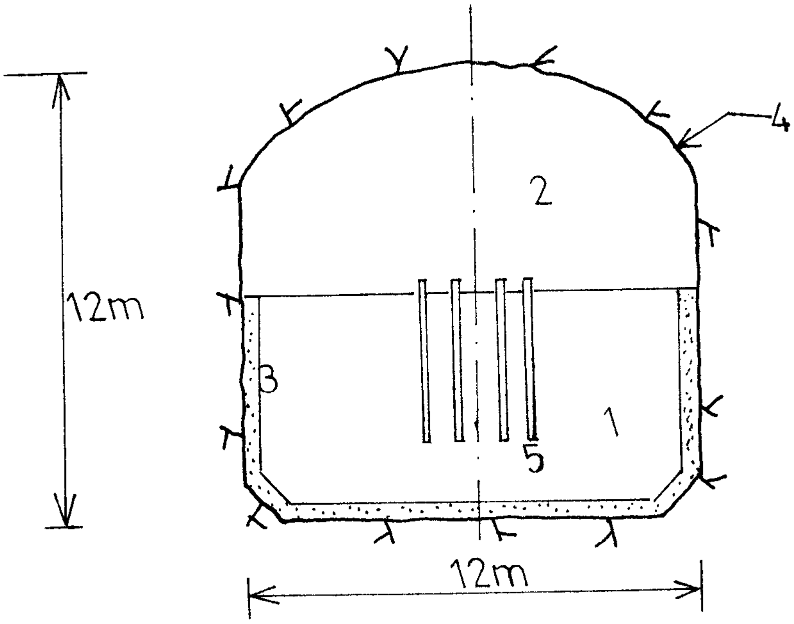
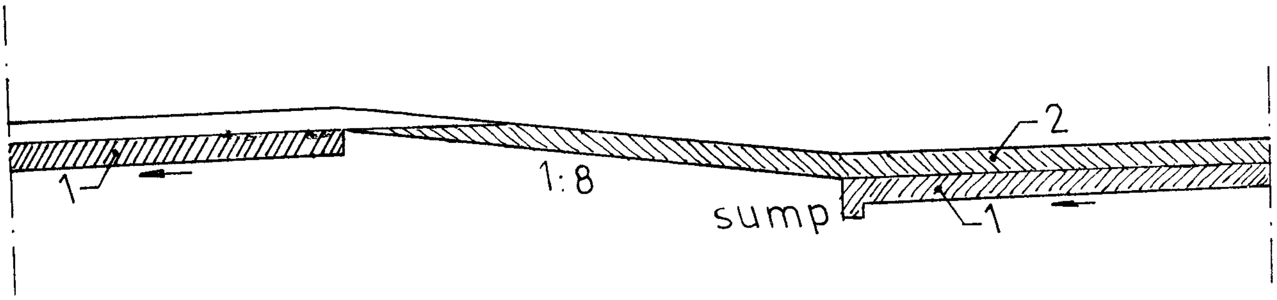


Figure 2-1. Suggested disposal of spent fuel in drillholes in a tunnel floor. (Not to scale; Aka (1976))



(a) Cross section of a tunnel



(b) Longitudinal section of a series of connected tunnels

Legend:
1. Containment earth fill with high ion exchange capacity
2. Fill of same earth as 1.
3. Drainage system with permeable earth
4. Shotcreted rock surface with water drainage
5. Steel sleeves for fuel elements

Figure 2-2. Earth containment repository concept panels with interconnecting smaller drifts. A bed of crushed rock material mixed with ion-exchange clay will be compacted in the lower portion of the tunnels. The level of the floors of the tunnel sections will gradually rise by including the connecting drifts. In the clay-fill, steel sleeves for holding the canisters will be emplaced in a square pattern. After loading of a tunnel section, the upper portion of this section and the connecting drift will be filled with the same clay-mix material.

The storage capacity of a panel with 2500 meters of connecting tunnels will be roughly 2000 tons of spent fuel. The heat generation at disposal of this spent fuel will be 2MW.

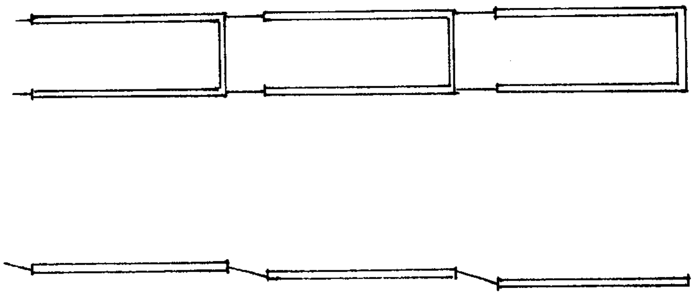
Two panel layouts that have been suggested are shown in Figure 2-3. According to these layouts, a panel could be composed of several parallel and perpendicular tunnels connected in series or in parallel.

2.4 Identification of principal processes

Figure 2-4 shows a schedule of the principal events relating to the geological containment of the waste following emplacement in the repository. These are shown in a bar chart form on a logarithmic plot of time in order to assist in the identification of possible sequences of containment mechanisms and the timing of coupled processes which affect the groundwater flow regime.

The waste composition was discussed in section 2.1 and details given in Tables 2-2 and 2-3. Analysis of the duration of the hazard defined in terms of the maximum permissible concentration in water to meet ICRP regulations will show that initially the hazard is dominated by the fission products which are heat generating and necessitate shielding. After approximately 300 years, the dominant hazard will be due to the actinides which persist indefinitely although their heat generation and radioactivity is small.

PANELS IN SERIES



PANELS IN PARALLEL

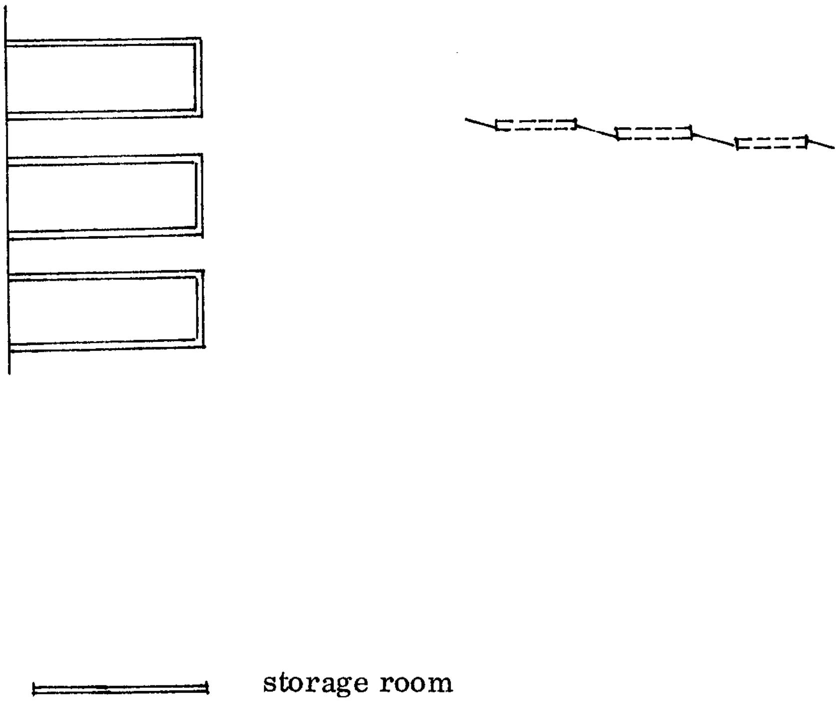
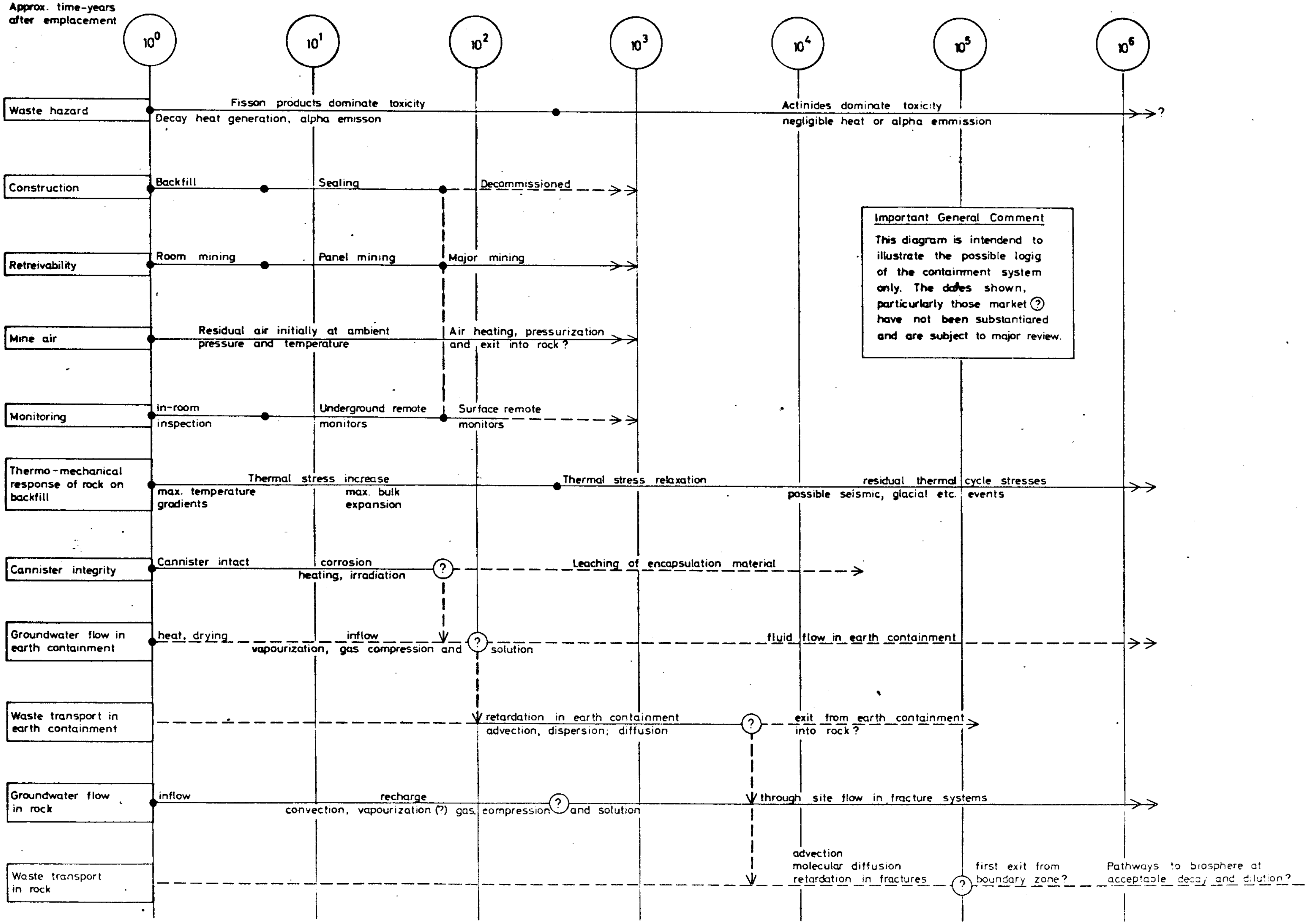


Figure 2-3. Panel layouts in the earth containment repository concept.



Important General Comment

This diagram is intendend to illustrate the possible logig of the containment system only. The dates shown, particularly those market ? have not been substantiared and are subject to major review.

Figure 2-4 Schematic Schedule of Events Associated with the Geological Containment of Radioactive Waste

A clay-fill repository concept was presented in section 2.3. Here we have simply noted the emplacement stages. In order to assist in maintaining room stability and minimizing perturbations to the joint systems, it will probably be advantageous to backfill the rooms as soon as possible. Sealing of the repository will also follow. Various sealing strategies are possible for isolating individual rooms, panels or the entire repository and the shaft, prior to decommissioning. These options will affect the monitoring program. If early backfilling and sealing are carried out, then in-place inspection of canisters for corrosion and sampling of groundwater will not be possible. However, remote monitoring will be possible initially at underground level, and finally from the surface facility. The backfill and sealing options will also affect the retrievability options. Initially, retrieval will be possible from the rooms. Later, progressively more elaborate mining procedures will be required.

The reference design concept will expose the room to ventilation drying of exposed groundwater from the host rock. If the backfilling is completed soon after emplacement, then little ventilation cooling or drying of the backfill material will occur. After backfilling and sealing, the remaining air in the pores will become thermally pressurized as a result of the decay heat, and recharge of the groundwater system will also occur.

It is expected that the thermo-mechanical analyses of the rooms will indicate maximum stresses due to temperature gradients after about one year. The maximum temperatures in the canisters, backfill and pillars and the associated thermal response will probably occur after about 10 years. Following this, cooling commences in the near field zone as the initial decay heat is conducted away. There is therefore, a long, slow period of thermal stress relaxation leading ultimately to residual stresses from the thermal cycle. The possibility of environmental factors,such as seismic events, reglaciation, etc., should also be considered to perhaps influence the thermo-mechanical response.

The canister material is a potentially reliable containment system. The time frames over which this can isolate the waste are unpredictable at this time, but with groundwater analyses and testing it may be possible to demonstrate a lifetime of several thousands of years for certain compounds. The canister material will be situated in a heated environment, subject to irradiation damage and corrosion, possibly enchanced by radiolysis of the groundwater. Ideally, the material should be able to achieve chemical equilibrium, although this may not be possible. It may be appropriate to isolate a local region around the canisters and backfill with an inert and initially dry sand in order to reduce corrosion.

The bentonite and till backfill for the rooms is a second, potentially reliable, containment system. This material will be subjected to a significant thermal cycle with temperatures near the canister/backfill interface possibly in excess of 100°C. Excessive drying of this material may leave undesirable fissures in the canister region after cooling. It may be appropriate for this reason to also provide an inert heat resistant granular material such as silica sand in the maximum temperature zone. This material could possibly be enclosed and surrounded by the containment backfill.

The pore water fluid in the backfill will be heated and subjected to natural convection forces and may vapourize locally. If the canister material corrodes, then this water could be in contact with the spent fuel and leaching of various contaminants may occur. (Since leach rates increase rapidly with increasing temperature, it will be clearly advantageous to attempt to design a canister material or enclosure which will prevent leaching during the thermal era.) It may be possible to demonstrate by laboratory experiments that strong retardation of the critical isotopes will occur in the backfill. Contaminant transport and dilution processes may include advection, dispersion and chemical diffusion. The prediction of these processes in granular media is likely to be much more reliable than in the case of fractured rock,partly, as a result of some previous work being available and partly, as a result of granular materials being much more amenable to realistic laboratory experiments.

The existing groundwater system will be disturbed by the repository construction, which will introduce a large sink into a system previously close to steady state. This inflow will probably provide an effective barrier against waste transport into the groundwater system, although the disposal of the pore water or vapour which has been in contact with the waste or the canisters will require consideration. The near field groundwater flow system, particularly after sealing, may include local natural convection in either joint systems or in individual features if they exist nearby. By designing sufficiently large rooms and backfilling at an early stage, it should be possible to avoid vapourization of groundwater in rock joints and thus avoid the problems of two-phase flow. The residual mine air after backfilling and sealing (probably from a minimum backfill porosity of 0.20) may be driven out of the rooms. The joint systems may therefore contain a mixture of water and air. The nature of this system will depend to a large degree on the relative length of time of the inflow/recharge era relative to the heat generating period of the waste. Ultimately, the far field groundwater system may return to a state similar to its initial state. The near field system will be permanently modified due to the existence of new materials and rock fracture.

The source mechanism is often simply referred to as leaching. Leach rate estimates vary widely and are highly temperature dependent. A more precise description is required in terms of diffusion, solution availability, flow rates and saturation limits. Subsequently, the waste could be transported by advection in the groundwater with consequent mechanical dispersion in the joint systems. Chemical diffusion in the groundwater will also occur to some extent. There is some potential for retardation of certain radionuclides. However, the state of the art for retardation prediction in joint systems is extremely primitive and is hampered by problems of testing large and representative rock samples.

If containment is considered within a cylindrical exclusion zone as suggested in section 2.3, then it is possible that certain radionuclides may start to escape at some time. By that time, substantial decay and dilution should have occurred and pathway analyses in the biosphere should demonstrate accepteably low levels of toxicity indefinitely.

In Table 2-4, we give summary descriptions of the principal processes which are associated with events discussed above. These have been classified as fluid flow, geochemical reactions and species transport, energy transport, thermo-mechanical responses, and source kinetics. These are then placed in time frames of the virgin state, the construction and emplacement period, the short term (30 to 1000 years), and the long term (1000 to 1000000 years).

We have also indicated the relative significance of these processes as they affect the containment system. The transient processes which occur in the short term period and appear in boxes (1.3), (2.3), (3.3), (4.3) and (5.3) are clearly significant and involve a very complex set of coupled processes. The long term processes appearing in boxes (1.4) and (2.4) are less coupled but involve geological time scales. The long term source kinetics in box (5.4) are both complex and of long duration. A more detailed discussion of these processes and the current state of the art regarding their physical or chemical description, predictability, data availability and the availability of testing and monitoring techniques follows in section 3.

In our review and recommended study program, we have primarily addressed the currently proposed earth containment room concept. It will be possible, within our study framework to consider certain other concepts. For

more significant
most significant

TABLE 2-4. BRIEF DESCRIPTION OF PRINCIPAL PROCESSES

	years VIRGIN (PRE-MINING)	30 CONSTRUCTION (PRE-EMPLACEMENT)	10^3 SHORT TERM CONTAINMENT	10^6 LONG TERM CONTAINMENT
FLUID FLOW	STEADY 1.1 Regional flow field	TRANSIENT 1.2 Flow into the excavation Impact of grouting and pumping	TRANSIENT 1.3 Air intrusion into host rock Backfill and sealing	STEADY 1.4 Regional fluid forecast Climatic changes (i.e., glaciation, erosion, tectonics).
GEOCHEMICAL	STEADY 2.1 Regional geochemistry	2.2 Impact of grout on geochemistry	TRANSIENT 2.3 Thermal degradation of rocks (phase and mineralogy changes), chemical diffusion, engineered geochemistry	TRANSIENT 2.4 Chemical diffusion and dispersion from source (sorption and reconcentration).
ENERGY TRANSPORT	3.1 Geothermal flux field	3.2 Drying of cavity by air circulation	TRANSIENT 3.3 Two Phase mixture, convective diffusion, transport in cavity and immediate vicinity.	TRANSIENT 3.4 Thermal modification of flow field. Near field cooling, far field subject to small amplitude thermal cycle.
ROCK MECHANICS RESPONSES	4.1 In-situ stress field as related to fracture permeability tensor	4.2 Local fractures (induced by excavation, rock bolting and mining sequences)	TRANSIENT 4.3 Thermally induced stress with quasi-static and creep cycles.	TRANSIENT 4.4 Near field thermal stress relaxation. General thermal expansion of far field.
SOURCE KINETICS	5.1 Background radiation field	5.2 Emplacement of precursive tracers	TRANSIENT 5.3 Species and source kinetics. Cladding and glass kinetics and dynamics, radiolysis, corrosion. Primarily fission product hazard.	TRANSIENT 5.4 Species and source kinetics. Cladding and glass kinetics and dynamics, radiolysis, leaching. Primarily actinide hazard.

instance, a concept currently under consideration in Canada for hard rock sites involves the use of waste-emplacement in drill holes in the floor of rooms. This containment system could be countered as a subset of the earth containment system. On the other hand, this floor drillhole concept allows the use of ventilation cooling for longer periods than the earth containment system. We can therefore quite easily modify our program of studies to include consideration of a drillhole design concept. General comments regarding the relative merits of the earth containment reference design concept relative to other developing concepts will be made in the final evaluation phase of this study.

3. STATE OF THE ART REVIEW

In this section, we review the available techniques for prediction of groundwater flow as it may affect containment, both within the repository rooms and the surrounding rock mass, over the full lifetime of the repository. As discussed in the previous chapter, the problem is in fact coupled with chemical, thermal, mechanical and geological processes.

The overall approach to this groundwater prediction problem will require the use of the most sophisticated field investigation data, in-situ experiment results, and laboratory experiments to develop and calibrate elaborate simulation models. These simulation models will then become the vehicle for prediction of the coupled processes in the long time frames. However, suitably reliable models and data gathering techniques are only available for certain of the processes individually, and techniques for their complete coupling are in their infancy if they are available at all.

3.1 Geological and geotechnical aspects related to groundwater flow

The development of testing procedures, simulation models and data availability for the reference repository concept involves two fundamentally different materials. The granular backfill material, involving compacted earth materials such as clay or other mixtures, is relatively amenable to laboratory testing and simulation,since the particles are sufficiently small and uniform to allow it to be modelled as a homogeneous or heterogeneous, possibly anisotopic, porous continuum. The bedrock on the other hand will contain fracture systems on a large scale with hydraulic properties which are not readily predictable.

The extraction of samples is very difficult due to the required size of a representative sample and the problem of avoiding disturbances to it. Some work is proceeding at the University of California, Berkeley on such a test procedure and will be discussed later. Mathematical simulation of fluid flow in fractured rock is currently approached by two techniques: (1) equivalent porous continuum models where the properties of the fracture system are modelled using statistical distributions, and (2) discrete models where the geometry of the fracture system is defined and analysed by a network technique. These models are solved for two or three dimensional problems using either finite-element or finite-difference techniques for either steady state or transient flow. A detailed review of these techniques was given by Wilson and Witherspoon (1970). A more recent summary was given by Witherspoon and Gale (1976).

In the following sections we discuss the application of these models to particular processes at various stages of the repository life together with comments on data availability and verification.

3.1.1 Regional hydrogeology

A regional hydrogeological model of the proposed repository site in its virgin or unmined condition will provide the reference state for modelling of subsequent phases, and its development and calibration against field data will serve to validate its long term prediction capability.

The hydrogeologic environment in the proposed Swedish sites can be subdivided into three depth zones for the purposes of modelling and discussion of field data:

(a) active zone
(b) intermediate zone
(c) inactive zone (or sluggish flow zone).

These zones are shown diagrammatically in Figure 3-1.

The active zone, in the absence of permafrost, extends from the ground surface and includes the water table (phreatic surface) in the permeable

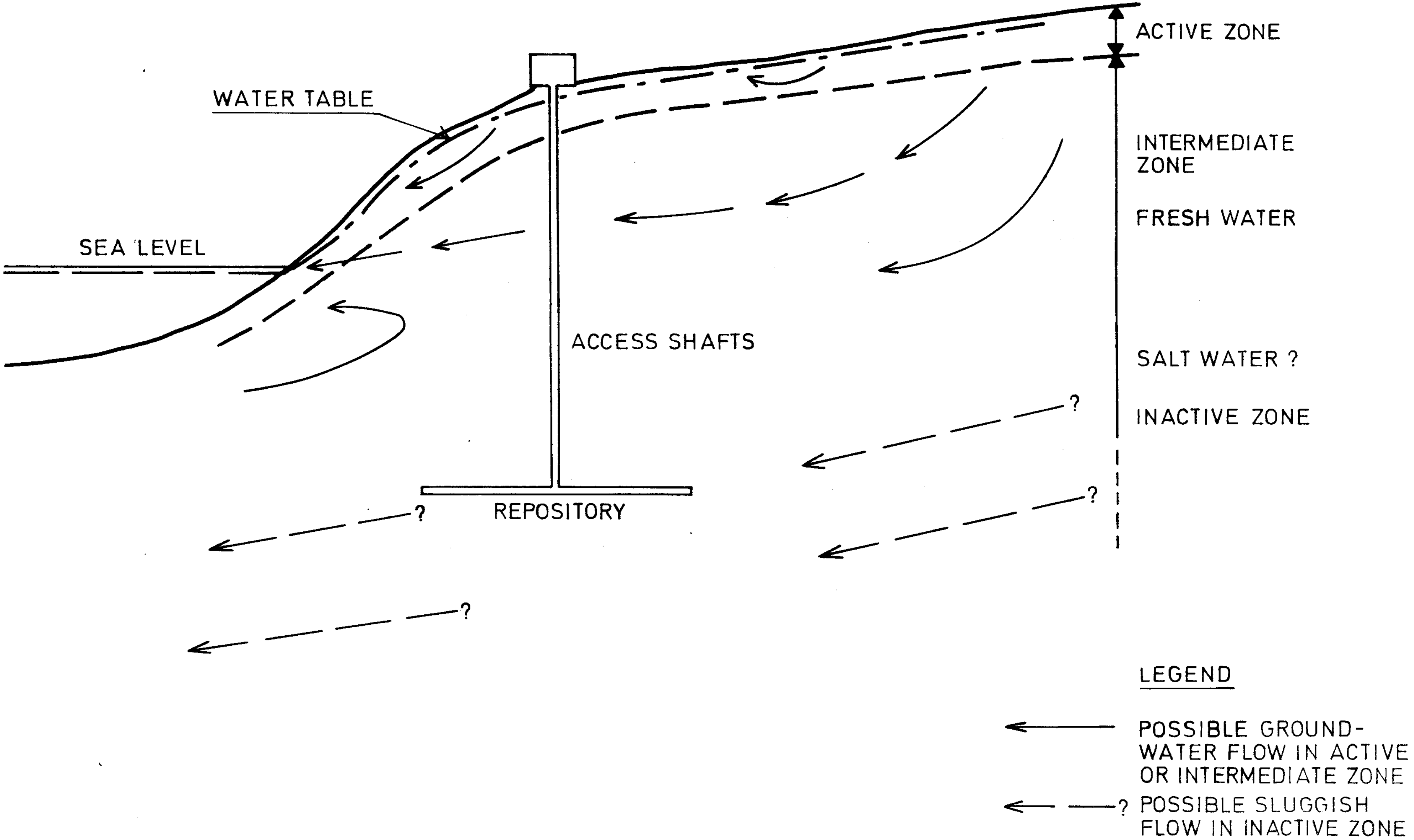


FIGURE 3-1. SCHEMATIC OF REPOSITORY GROUNDWATER ZONES.

overburden and upper bedrock. The upper bedrock would be expected to have appreciable fracture systems and joint systems which are permeable. The overburden can include surficial layers of moss, peat, glacial till, glacio-fluvial of glacio-lacustrine deposits, composed mainly of gravel, sand, silt or clay. Fault systems with relatively large permeabilities may occur in this zone. Permeability values in the active zone are typically greater than 10^{-5} m/sec. Groundwater circulation in the active zone is generally quite rapid and shallow, with numerous recharge and discharge areas affected by evaporation, transpiration and precipitation.

Groundwater levels will fluctuate due to variations in recharge and in the stress field in the rock. Stress field variations can be caused by changes in the earth´s gravity field. This effect has been observed in the Fennoscandinavian bedrock, and is analogous to tidal effects in oceans. The elastic reaction of the earth´s crust to the influence of the moon and the sun will somewhat change pressure conditions in aquifers and rock fractures. Also barometric pressure changes will cause fluctuations in water tables. Whether or not such cyclic changes of groundwater pressure conditions may have any appreciable effect on the flow regime around a repository is not fully understood at the present time.

The active zone groundwater will probably have detectable tritium indicating age less than 25 years. Isotopic age dating is discussed further in section 3.2.1.

The <u>intermediate</u> zone is situated below the active zone with permeabilities generally less than about 10^{-7} m/sec. Fault systems may extend through the intermediate zone and give rise to higher permeabilities locally. We could define the intermediate zone as having no detectable tritium but having detectable carbon 14 (see section 3.2.1). Initial field data for proposed repository sites indicate saline groundwater. A fresh/salt water interface, or transition, will probably exist in the intermediate zone. Circulation may occur above and below this interface and probably be stable, or at equilibrium, in an essentially steady-state system. Annual perturbations may not have significant effects.

The inactive zone is a desireable zone for repository siting. It could be defined by age dating as possessing no detectable carbon 14 and certainly no detectable tritium. This zone should have very low permeabilities, possibly less than 10^{-8} m/sec with very low hydraulic gradients, possibly less than 10^{-3}. Singular features or faults may extend into the inactive zone, but low hydraulic gradients, mineral infilling and high in-situ stress should prevent significant flow. The fracture system will probably be fully saturated but the porosities and storage should be very low.

An equivalent porous continuum model will probably be appropriate for the regional groundwater flow model. Many two- and three-dimensional computer programs exist which can simulate a steady-state flow field. Two-dimensional models are of course much easier and less expensive to use. Initial data suggests that saline groundwater will occur in the zones proposed as possibilities for repository siting. The region of interest will probably extend above the salt/fresh water interface. This interface therefore should be included in model studies of the regional flow field. Salt water intrusion models which include a density change across the discrete interface exist. Because of mixing, the interface may not be distinct. Depending on the location of the interface relative to the repository, the models that take into account transient but non-mixing interfaces may be adequate.

The models discussed above are for fully saturated materials. Some current research is in progress for the testing, description and modelling of partially saturated materials. The virgin state in the inactive zone will probably be sufficiently saturated to permit this assumption for simulation purposes. However, after emplacement, air will be present in the fissures. Work on two-phase flow in fractured materials is only in the initial stages of development.

By applying appropriate boundary conditions on groundwater potential and recharge fluxes and extensive borehole data to derive equivalent statistical permeability and porosity parameters, the model should provide an overall flow field including circulation both in the fresh water and salt water regions. This model could then be used to investigate possible perturbations to the flow field by repository construction and operation. Use of these models need not await acquisition of all of the necessary field data from site specific studies. Intensive studies based on parameter analysis (sensitivity analysis) would be appropriate for the near future. Simulation models for bedded aquifers are frequently simplified to two dimensions in the plane of the aquifer with discharge or recharge terms included for flow perpendicular to that plane. In this way, very large models can be developed. Layered two-dimensional models are also used in appropriate geology. In the case of the regional modelling, layered models will probably not be appropriate. For steady-state analyses, the use of three-dimensional models may be manageable, depending on the complexity of the hydrogeological system. For parametric studies of perturbations to the regional system, it will probably be appropriate to develop sub-structure models, particularly if these pertrubations require transient analysis. Various options are available. Two-dimensional models of flow in a vertical plane could be calibrated for out-of-plane response against the three-dimensional model. This model could be large and could certainly extend to the surface in order to handle possible long term environmental changes. Locally, either small three-dimensional, two-dimensional plane flow, or possibly axisymmetric analyses could be used for transient responses in the near field region.

Variations on a porous continuum model are available and may be applicable to the near field flow problem. If the rock blocks are porous, then many models assume that the blocks provide most of the storage while the fractures are the flow channels. These principals are then used to develop a permeability tensor to use in a continuum model. This approach is dependent on determining the fracture apertures and distribution. Attempts have been made to obtain this information from borehole injection test data, photographic techniques and elaborate packer tests in multiple injection boreholes.

It has been suggested that discrete models of the fracture system should be used in the near field region. Theoretical models exist for discrete fracture systems in which the fractures are the principal conductors and the rock mass is rigid (Wilson and Witherspoon 1970; Wittke, et.al., 1972). This model has been used for parametric studies on the effects of fracture size and the effects of underground opening size on regional flow. The decision on the required degree of discrete fracture modelling is flexible from a mathematical modelling point of view, but the availability of reliable data will severely limit the application.

The above techniques for incorporating discrete fractures into a continuum model may also be useful for modelling the response of the final sealed tunnel network in which the tunnels could be treated as discrete fractures with specified conductivities. The convectivity which the rooms introduce in either a pure continuum or a continuum with certain specified major fractures could therefore be simulated.

Although, ideally it may be desirable to model discrete fractures locally, the overall objectives of the groundwater simulation effort could probably be met by making certain simplifying assumptions for permeability/conductivity in the near field and only use the results at a minimum distance of say 50 meters from the rooms. The gross flows within that region may be mainly controlled by the external response, and local variations due to previous or induced fractures may not affect the overall containment demonstration. Witherspoon and Gale (1976) argue that the lack of data for discrete models is no longer a valid criticism for this dismissal since improved borehole techniques are available for three-dimensional mapping of the joint geometry and hydraulic system. In the case of a radioactive waste repository however, extensive drilling may not be permissible due to problems with sealing the drill holes. The extent of the drill-hole sealing problem could also be quantified by considering boreholes as discrete flow paths in a continuum model as discussed above.

If such studies prohibit extensive drilling, then remote fracture mapping techniques will be required. This may be possible through various transient tests from an in-situ experimental station in the proposed repository site. Groundwater withdrawal tests have been considered, but the techniques for reliable withdrawal of the expected small quantities of water are not yet sufficiently developed to be of value. Isotope tracer tests have also been suggested. Although little work has been done in the use of either single borehole dilution methods, or two-borehole tests in fractured rock systems, the methods appear to have potential. However, they may have low reliability as indicators of lack of connectivity, but possibly higher reliability, or acceptability, as indicators of positive connectivity. Consequently, for containment arguments they may only be valuable in the negative sense.

Injection tests for steady state or non-steady conditions are well developed for porous systems, but need further refinement for fractured systems. Pulse tests are, apparently, unproven for fractured systems.

The above testing techniques may yield useful data on near field hydrogeology. However, their use in validating a regional flow model will be rather limited due to the slow response times and discontinuity of local features. These test results may well be of value in assessing inter-room flow inside the repository.

3.1.2 Groundwater inflow and grouting

Investigations of groundwater inflow to tunnels and rock chambers in Swedish precambrian bedrock are limited to the active zone of groundwater flow because most of the tunnels and caverns are constructed at depths less than 100 meters. The rock in this area can have a lot of fissures, and therefore, the amount of leakage depends on the extent of rock fissuring. For heavily fissured rock, the "effective permeability" will be around 10^{-6} m/sec or higher and, for extremely competent rock, the value will be around 10^{-8} m/sec. For rock chambers at great depths, the value will probably be less than 10^{-8} m/sec, if major systems of fissures are avoided.

The problems of grouting in connection with rock chambers for radioactive waste repository are divided in two parts, one of which concerns the long term stability of grouting material and one of which concerns the sealing effect. The long term stability can be divided in several parts in that the grouting material shall have chemical stability, including of course minimal water solubility, and physical stability, so that no cracks or creeping will reduce the sealing effects. Due to all of these factors, it is clear that the material shall be a so called "natural material", and not a chemical material like a plastic product because of the lack of knowledge of the stability with time. New products for grouting material, for example silica with long term stability, can be developed in the future and change this premise. Today, however, the only natural products used by the grouting companies are cement and bentonite. For cement slurry as a grouting material, the lower limit of the joint width which can be successfully treated will be about 0,5 mm. With special fine-graded cement material, the penetration ability will increase such that a joint width of approximately 0,1 mm can be grouted. A problem with cement will be shrinkage and creeping. In order to improve these characteristics, a swelling material is added. However, more study of the long term stability due to this swelling material is required. The long term stability of bentonite in

Swedish precambrian bedrock may be good, but the sealing effect can be damaged by high pressure gradients and water flow.

The grouting program for the site should be based on geological data, with the goal of sealing to both reduce the inflow and outflow of water, and not simply the inflow as is the usual case for rock chambers. The measured flow through jointed rock for tunnels up to depths of 50 meters shows that the "effective permeability" changes from about 10^{-6} m/sec to 10^{-7} m/sec due to grouting. The difficulty with sealing joints increases with decreasing joint width.

3.1.3 Modelling of groundwater inflow and recharge

In the discussion on the problem definition, it was suggested that an inflow or recharge era may exist for possibly several hundreds of years. This feature may provide an additional containment mechanism and should therefore warrant detailed investigations. In the previous section, general comments on inflow were presented. In this section, we briefly review simulation modelling techniques for extrapolation purposes and for use with site specific data as it becomes available.

Initially, during construction and prior to complete backfilling with earth materials, the rooms will be ventilated. The airflow will tend to dry the rooms. The precise prediction of the extent of drying into the fissures is presently not possible and probably of little value. However, ventilation simulation models exist which can include simple heat transfer coefficients for air/wall interaction. These models could be used for order of magnitude drying and atmospheric groundwater removal estimates. This may be important since the drying effect may mask or at least interfere with groundwater inflow measurements.

A transient flow model, possibly used as a sub-structure model of the regional flow model discussed in section 3.1.1, could be developed to simulate the inflow while the repository rooms are open. Such models are readily available and can be calibrated against flow data of the type discussed in section 3.1.2, plus other more refined techniques.

The transient model could then be modified to include the effect of backfilling the rooms and the subsequent recharge period. This model should handle the combined flow field in the backfill material and the host rock. The material properties of permeability and porosity for the granular backfill can be reliably estimated for the isothermal condition. The thermal effects will require recognition since they will introduce changes in the material properties and convection currents. In addition the mechanical response will also have an effect. Various coupled thermal/consolidation models exist for fully saturated flow, (Sykes, Lennox and Charlwood, 1972), which for instance could simulate the behaviour as a linear thermoelastic porous continuum and include natural convection terms. However, the value and reliability of such models in the current context in the light of various non-linear effects, due to the bentonite, partial saturation and ill-defined higher temperature behaviour and possible two-phase flow, will require further assessment. The most reasonable approach is probably to use constitutive laws developed from laboratory experiments in conjunction with the field equations employed in the simulation procedures.

The duration of the groundwater inflow period will be very dependant on the porosity of the clay backfill, on the permeability and porosity of the rock mass and on the extent of new fractures and drying fractures. The response of the fractured rock system will in this case be sensitive to the modelling detail in the near field. Parametric studies, explicitly recognizing the uncertainties, should therefore be made, and then can be linked to pressure transducer measurements in the backfilled rooms. The uncertainty in recharge predictions will therefore be progressively eliminated as time progresses after emplacement.

The recharge process will tend to drive out the residual air both in the backfill material and also where it has been introduced into fractures. Subsequently, this "air bubble" will tend to rise to the surface. This phenomenon is similar to the behaviour of natural gas in a fracture reservoir or the air in a compressed air energy storage system. This is discussed further in section 3.1.4 below. This is a currently active research field and some modelling and flow laws should be available for this study.

The pressure build-up in the repository should ultimately lead to hydrostatic equilibrium. At a depth of 500 meters, pressurization to approximately 50 bars will occur. If the fluid/air boundaries are mobile and can overcome possibly high capillary forces in fine fissures, then an air volume reduction by a factor tending towards 50 should be expected. This will therefore lead to almost saturated conditions.

3.1.4 Groundwater flow within the repository in the long term range

In order to establish the feasibility of achieving a high degree of isolation of radionuclides from the biosphere through the "deep repository in crystalline rock option", it is going to be necessary to construct a long term isolation environment within the mined cavities. To achieve containment for tens of thousands of years or longer and to insure that the release rate of radionuclides beyond this time will never be large, a containment system must be constructed primarily of geologic materials rather than of man-made materials such as metal or concrete. No matter what investigations of the natural hydrogeologic system are conducted in zones beyond the cavity, the level of uncertainty in predictions of radionuclide migration from the cavity towards the biosphere may be large.
It will require many years and perhaps decades of study at specific sites before the magnitude of the uncertainty can even be evaluated in a very meaningful manner. At present, one cannot even claim that the probability of finding good sites in crystalline rock at depths of less than 500 to to 1000 meters is very high. By "good sites",we refer to sites that will

within a high degree of confidence, provide containment in the natural hydrogeologic system beyond the deformation zone associated with the mined cavities. It is imperative, therefore, that an adequate conceptual design of an engineered hydrogeological-geochemical system (often referred to in this report as the earth media) for the cavities be attained so that the feasability of achieving long term isolation can be analysed quantitatively. If sites are located in the next few years or decades that offer adequate natural long term containment, all components of the engineered hydrogeological-geochemical system may not be required; or preferably, they could be used to achieve greater redundancy.

The purpose of constructing a carefully designed hydrogeological-geochemical environment in the cavities is two-fold. Firstly, it is to provide a much longer period of radionuclide containment than would otherwise be the case. Secondly, it is to reduce the eventual rate at which radionuclides will migrate from the cavity towards the biosphere. To achieve these two objectives,it is necessary to accomplish the following:

(1) the flux of groundwater moving past the waste canisters must be reduced to very small rates;

(2) the velocities of groundwater flowing from the interior of the cavities towards the biosphere must be extremely small;

(3) the rate at which radionuclides can move by molecular diffusion or hydraulic transport from the interior of the cavity (where the canisters are located) to the periphery of the cavity must be reduced to rates well below those that would occur in a single phase aqueous (i.e. non-porous medium) system. This can be accomplished by providing tortuosity of microscopic transport paths (i.e. decreasing coefficients of molecular diffusion) and by chemical retardation.

The key element in any engineered hydrogeologic-geochemical system will probably be carefully constructed zones that include one or more layers of very low permeability materials. For illustrative purposes in this discussion, these zones will be referred to clay layers. If layers of clay are emplaced in the cavities at some distance from the canisters, but totally surrounding the canister zones, a protective zone of extremely low permeability material may be obtained. This would be the case if it can be insured with reasonable reliability that the clay does not become cracked or jointed prior to achieving full saturation during the period of groundwater inflow. Hydraulic conductivities in the order of 10^{-10} cm/sec or lower can be reasonably anticipated (for purposes of illustrative calculation) for wetted, highly confined clays of this type. To provide an indication of the groundwater velocity that would be expected in this clay zone, a hydraulic gradient of 10^{-2} will be assumed. Hydraulic gradients at great depth in slightly fractured crystalline rock will most likely be lower than this. Our choice of 10^{-2} is therefore conservative.

Velocities can be computed from relation, $V = \frac{K}{n} \cdot i$

where K is the hydraulic conductivity, n is the porosity and i is the hydraulic gradient. Using the above mentioned values (and a porosity of 0.2), we obtain a velocity of 1 centimeter in 5000 years. Thus, a clay layer just 2 meters thick would produce a cross-flow travel time of 1 million years. It is conceivable that for short periods of time during the wetting phase much larger cross gradients could occur. Nevertheless, at such low hydraulic conductivity, the groundwater velocities in the clay would be very small. It is evident that if an uncracked clay zone can be established in the repository, hydraulic transport of radionuclides through the clay layer from the canister zone towards the periphery of the canister would be a relatively insignificant process. Not only could a high degree of waste isolation achieved by the clay layer (it must be continuous around the canister zone), but also a high degree of predictability could be achieved; this is provided that the clay layers are emplaced properly, and provided that the clay does not greatly deteriorate under the influence of thermal effects and geochemical changes in the pore water caused by thermal effects and gas dissolution during the period of groundwater inflow to the earth media.

The hydraulic conductivity of saturated confined clays can be measured in the laboratory with existing technology. It is reasonable to anticipate that predictability of hydraulic conductivity values for clays under the conditions that would exist in the tunnels could be achieved within a factor of 5 (half an order of magnitude or better). Thus, if proper emplacement of a clay zone several meters thick could be achieved, hydraulic transport as a mechanism for radionuclide migration from the cavity would be effectively eliminated. Greater protection from the effects of earthquakes or glaciation could be achieved by use of thicker clay barriers.

The reduction of hydraulic transport rates to such very low rates however, would not, in itself, insure long term isolation of the radionuclides from the biosphere. It is necessary to consider a second transport process, known as molecular diffusion. Molecular diffusion will cause dissolved radionuclides to migrate from the waste canisters through the geologic materials in the cavity and then beyond into the fracture network in the crystalline rock. This migration occurs due to the concentration gradient directed outwards from the canisters as the spent fuel mass slowly dissolves (or as ions diffuse out of the matrix). Under conditions of extremely slow hydraulic flow of pore water, molecular diffusion is the dominant process by which radionuclide migration occurs in saturated porous media. The importance of this process and its role in the consideration of the groundwater system is discussed in sections 3.2.5 and 3.2.7.

Data availability

To proceed with a design of an engineered hydrogeological-geochemical system within the repository tunnels,it will be necessary to have information on the hydraulic conductivity, porosity, and minerology of geological materials. For preliminary designs, however, it should be possible to obtain useful estimates from grain-size data and data from hydraulic or consolidation tests on these materials under conditions that may not be specifically analogous to the conditions that will exist in the repository.

Much more crucial to design of the engineered hydrogeologic containment system is the behaviour of clay minerals under high temperatures and altered pore water chemistry,and under conditions of bombardment by products from radioactive decay. Since the main purpose of placing clayey materials in the cavity will be to achieve radionuclide containment, it is necessary that reliable predictions be made with regard to the behaviour of the materials during the high-temperature and compressed air phases of the repository history. It is well known that clay minerals can undergo crystallographic and compositional changes when subjected to elevated temperatures. If these changes cause the clayey deposits to become cracked, their integrity as a containment medium may be lost. Ruptures or even micro-fractures in emplaced clay zones could significantly increase the hydraulic conductivity of these zones. Compositional and crystallographic changes in clays or other minerals will change the capability of the materials for radionuclide retardation. This effect could be very serious, since it could be the retardation capabilities of the emplacement materials in the cavity that provide the main bases in predictive models for judging the degree of containment provided by the facility. Preliminary discussions with research workers in this field suggest that temperatures of 200°C or even lower cause major changes in some types of clayey materials. It has been suggested that temperatues below about 150°C or 125°C have much less influence on the physical and geochemical nature of these materials.

One of the most important factors in the design of the hydrogeologic-geochemical containment environment in the cavity may be the arrangement of the geologic materials in a manner so as to insure that the clayey zones do not encounter temperatures above some critical level. It will probably be inadvisable to emplace clayey material close to the spent fuel rods. Relatively inert, thermally resistant geologic materials such as silica sand may be suitable for this purpose. In terms of evaluation of the containment capabilities of hydrogeologic systems within the repository, there is a necessity for quantitative data on the thermal stability of clayey materials at various temperatures. To our knowledge, adequate data of this type are not available at present. If the emplaced clayey materials become wet as a result of groundwater inflow during the period of high heat flux, the problem of clay mineral alteration at elevated temperatures becomes even more complex. It would appear that there is a need for intensive laboratory studies of the behaviour of potential emplacement materials of clayey texture under conditions of variable temperature water contents, and pore water chemistry. In addition to the direct effects of temperature, the physical nature of the earth materials may be greatly affected by changes in the chemistry of the pore water. These changes may occur because of the temperature changes, or because of changes in dissolved gas concentrations caused by air compression during groundwater inflow. This is discussed further in section 3.2.4.

Predictive capabilities

As mentioned above, at present there appears to be little capability available for prediction of the mechanical behaviour of clayey material within the cavity under high-temperature conditions. This is not a problem that is well suited for simulation studies. It would appear that the necessary information must come from empirical laboratory-based investigations.

The engineered hydrogeological-geochemical environment within the cavity would be designed for the purpose of achieving long term containment of radionuclides and for limiting radionuclide leakages over extremely long term periods to very low rates. The suitability of any proposed design will rest on the results of simulations of hydraulic conditions and radionuclide transport under various imposed boundary conditions. For this purpose,two-dimensional groundwater flow and solute transport models will be required. These models must be capable of accommodating large contrasts in hydraulic conductivity between zones of different geologic materials, small thermal gradients, molecular diffusion, and mass loss due to radioactive decay. Since the system would be designed to produce very low groundwater velocities, the effect of mechanical dispersion of radionuclides within the repository would probably need not be included in the simulation scheme.

For simulation studies of the wetting phase of the earth environment that will occur during groundwater inflow, it would be necessary to model two-phase flow (air and water) under conditions where the air pressure becomes very high. The fluid driving gradients will also be extremely large. It is doubtful whether adequate models are available for simulation of two-phase fluid under such unusual physical conditions.

3.1.5 Effects of long term hydrogeological and gross geological/ environmental changes

The simulation model development discussed in 3.1.1 and in subsequent sections can, theoretically, be used to simulate the very long term conditions. The period of interest for contaminant transport will probably begin several hundreds to thousands of years after emplacement, at a time when radionuclides could conceivably exit the backfill material. At this time, the rock mass should be well into the cooling phase and it will be necessary to recognize residual thermal cycle effects. Another requirement will be to demonstrate that no mechanisms exist for the transport of radionuclides through the earth material into the rock mass. For small fissures, it should be possible to demonstrate this. If large fractures occur, then a potential for backfill transport may exist, and analysis and experimental work may be required. This question can probably best be handled by considering single fractures and general simulation would only be used to define the boundary conditions.

At this stage, the principal use of simulation models would be to provide semi-quantitative answers to postulated hazards. These could include gross geological environmental changes, and other possible containment failure mechanisms.

We now give a brief review of various mechanisms which have been suggested as having possible loss of containment consequences. These have arisen in the course of the U.S., Canadian and other repository studies.

Potential mechanisms of containment failure, that may result from gross geological changes over a period of 250000 years, involve both possible and highly improbable phenomena. Possible phenomena include weathering, erosion and glaciation. In the category of highly improbable phenomena, consideration must be given to volcanic activity, faulting, and meteorite impact. Apart from weathering and glaciation, assessments of erosion and the three highly improbable phenomena have been made in the context of a repository in bedded salt in the south-western United States (Claiborne and Gera, 1974). These results and the methodology employed would provide a framework of thought for a similar assessment of any proposed repository site in Sweden. All of the phenomena cited above, excluding meteorite impact, are site or regional specific.

Meteorite impact is a random process, and will produce a crater with a depth of approximately one-third of its diameter. Claiborne and Gera have estimated the frequency of impacts of giant meteorites in Quaternary time as 10^{-13} per km^2-year. Assuming a repository facility depth of 600 meters, it would take a crater with a diameter of approximately 2 km to cause an instantaneous release of a part of the emplaced radioactive waste. The probability of formation of a crater 2 km in diameter or greater is about five times lower than the probability of formation of a crater 1 km in diameter. Assuming a general repository area of 10 km^2, the probability of a catastrophic meteorite impact, capable of causing some atmospheric release of radioactive waste, is about 2×10^{-7} per year in a one million year period. Based on crater formation data for nuclear explosives, Claiborne and Gera estimate that less than 1% of the waste materials in the repository would be released to the atmosphere, with the remainder being exposed to groundwater action. The consequences of these events were then analyzed in the context of contamination of the biosphere including the migration of radionuclides in the groundwater.

Volcanism is not a random process, as it is generally confined to the proximity of boundaries between crustal plates and is commonly associated with well-defined tectonic features. Claiborne and Gera estimate that the probability of volcanic activity being initiated in a tectonically stable area, with no magmatic manifestations, must be significantly lower than the probability of the formation of a great fault. They also conclude that the consequences of a volcanic event would be less serious than those for the impact of a giant meteorite.

Claiborne and Gera (1974) estimated that the probability of a large fault intersecting a repository in the Delaware Basin in the south-western United States is 4×10^{-5} in any one million year period. However, the probability of containment failure through faulting is supposed to be lower than the probability of faulting, but cannot be estimated quantitatively. If containment failure would occur for one fault in every one hundred faulting events, than the probability of radioactive material release would be of the same order of magnitude as for the impact of a giant meteorite.

Based on the analysis of Claiborne and Gera (1974), and in the context of a repository facility at a depth of 500 meters or more in granitic rock in Sweden, erosion can be reglected as a potential mechanism for containment failure for erosion rates of one centimeter or less in one thousand years. This rate of erosion was reported in the document entitled "Spent Nuclear Fuel and Radioactive Waste" (1976, p.55).

Gneisses and granites,being high in silica content,are very resistant against weathering in the climate in this part of the world. Clear evidence of this, are outcrops of rock which were scratched about 10000 years ago by the glacial ice and which have still scratch marks on them. Alteration of feldspars to caolinite and laterite earth existing in tropic climates develops very slowly and never reaches a depth greater than 50-100 meters in a bedrock free from major cracking. Heating of the rock to 200°C should not give rise to accelerated chemical weathering of quartz and feldspar minerals. However, one has to check the risk of spalling of the rock material close to the rock tunnel walls and roofs due to thermally-induced stresses in the bedrock. This analysis need is based on experience with chambers designed for the storage of heated oil and oil products.

During the million of years of the history of the earth in which we now live, called Quarternary time, there have been at least 4 periods of glaciation with intermediate interglacial periods. The duration of these is several 10000 of years, and we are probably now in an interglacial period which will be replaced by another glaciation. During the glaciation periods, an ice cover of more than 3000 meters compressed the Swedish bedrock. After melting of the ice, the bedrock began to rise slowly. The total amount of rise is at least 300 meters and is still continuing. Movements seem to occur along the old regional fracture zones. It is interesting to note that the relatively large blocks of undisturbed rock which exist in the precambrian shield have withstood several glaciations without major fracturing or cracking.

Failure and crack zones in the precambrian shield can extend laterally to hundreds of kilometers. Undoubtedly there exist failure zones in the Fennoscandian shield, along which tectonic pertubations have occurred several times during the history of earth, and one could not disregard that some of them have also been active after the latest glaciation (about 10000 years ago).

The chance of finding a stable rock portion is good with regional tectonic analyses (possibly using satellite pictures) indicating failure zones. The existance of undisturbed sedimentary rock and soil layers will be of great value, as well as detailed analyses of failure and crack zones that may be circumferential to undisturbed massive blocks of rock. Wide brecciated zones and zones with altered schistous rocks are judged to have a damping effect on the block of rock in the event of earthquakes.

3.2 Geochemistry

3.2.1 Use of environmental isotopes

In evaluating the groundwater conditions at potential repository sites, groundwater constituents known as environmental isotopes will be useful. The main isotopes of interest in this regard are tritium, carbon 14, oxygen 18, and deuterium. Tritium and carbon 14 can be used as indicators of groundwater ages. Oxygen 18 and deuterium can, in favourable circumstances, be used as indicators of temperature conditions that existed at the time the groundwater was recharged from the atmosphere (rain and snow) to the subsurface flow system. Profiles of oxygen 18 and denterium as a function of depth can sometimes be used to identify periods of major climatic shift, such as occurred when the climatic regime changed from Pleistocene conditions to the warmer post-Pleistocene conditions.

Since the main objective of the deep rock repository is to achieve isolation of radionuclides from the biosphere, it is essential that as much evidence as possible be obtained for evaluation of the groundwater flow conditions. If it can be shown on the basis of isotopic evidence that the proposed repository level is located in a zone of very old groundwater, much will have been achieved.

Use of environmental isotopes to establish that a proposed repository level is situated in a zone of very old groundwater will be hindered by two major difficulties:

(1) In test boreholes at proposed sites, it will be difficult to obtain water samples that are truly representative of the natural waters in the fractured zones adjacent to the boreholes;

(2) Interpretation of data will be complicated by the fact that the proposed repository sites are below sea level at coastal locations.

It will be necessary to establish that the drilling water has been removed and that waters from other depth zones are not "contaminating" the samples.

Special packer isolation systems will need to be used in order to isolate zones from which samples are desired. Fortunately, only small volume samples are necessary for analysis of tritium, oxygen 18, and deuterium. Thus, it should be possible even at considerable depth in slightly fractured rocks of low permeability to obtain samples of adequate size for analysis of these isotopes. Analyses of numerous samples from each depth zone collected at different times may be necessary to establish representative values for undisturbed conditions.

For analyses of carbon 14 samples, several tens of liters of sample volume are normally required. During sampling, excessive interaction with borehole gas should be avoided. There is distinct possibility that it may not be technically feasible in the immediate future to obtain adequate carbon 14 samples from drillholes in slightly fractured crystalline rock with very low permeability. At present, it appears that the main limitation in the use of environmental isotopes for evaluation of groundwater conditions at proposed repository sites lies in the difficulties associated with sample collection.

3.2.2 Geochemical conditions during the pre-mining period

In order to develop predictions regarding the mobility of radionuclides leached from the wastes into the hydrogeological environment, it will be necessary to know the chemistry of the groundwater along the potential migration paths. The groundwater chemistry is an important factor because: (1) it can exert a strong influence on the type (species) and concentrations of radionuclides that will go into solution as the wastes are leached during contact with groundwater; and (2), it can, to at a major extent, control the physiochemical nature of the rock surfaces exposed along fractures or joints. The physiochemical nature of these surfaces (including their coatings) will play a major role in the mobility of the radionuclides in the hydrogeologic environment. To develop predictions regarding long term radionuclide migration rates from the repository towards the biosphere, it will be necessary to conduct highly controlled radionuclide partitioning experiments involving appropriate radionuclide-spiked aqueous solutions and appropriate rock materials. It will not be possible to design experiments that are relevant to field conditions unless the chemistry of water that will enter the repository and the chemistry of water further away from the repository are known. If metallic cladding is used as a containment medium, knowledge of the natural groundwater chemistry will be necessary for evaluation of corrosion rates. This information will also be necessary for analysis of the leaching rates of the spent fuels if the metallic cladding is ruptured.

State of knowledge

Our review of the literature has provided no direct information on the natural chemistry of groundwater deep in granitic rocks in plutonic masses in any area of the world. There is considerable information on groundwater chemistry in shallow hydrogeologic zones (i.e.$<$ 100 m) in granitic or granodiorite rocks. Whether or not this type of information has much relevance to hydrogeologic conditions at considerably greater depth remains to be determined. In this regard, the problem centers around the fact the chemistry of groundwater depends on the initial conditions in its areas of recharge; on the minerals that it encounters during migration from its recharge areas to the point of interest (i.e. to the repository site); on the rates at which reactions between the water and the minerals occur; and, on the travel times. It is well known that many of the important reactions that can occur between groundwater and granitic minerals (such as quartz, feldspars, and other aluminosilicates) are extremely slow (i.e. the kinetics are very sluggish). Thus groundwater that has reacted with granitic rock surfaces over periods of years or tens of years will likely be much different than water that has had thousands or tens of thousands of years of contact time. Unfortunately, the data that has been published on the geochemistry of groundwaters in non-geothermal, granitic environments generally relates to waters that are definitely young, or appear to be young, or at least cannot be proven to be very old.

A further complicating factor for the proposed repository is the fact that present plans indicate the repository will likely be located at depths well below sea level in a coastal area. If this is the case, normal concepts of water chemistry evolution in fractured granitic rocks may not be applicable. It is reasonable to expect that the water in the repository zone will be brackish or saline in composition. The salts may exist in the water as relic salts from episodes of Pleistocene salt water occurrences in inland areas. On the other hand, salts may occur at the depth of the repository as a result of the normal conditions of dynamic equilibrium, whereby saline water exists below the fresh water zone in coastal areas. Prediction of the geochemical consequences of interactions between saline water and fracture surfaces in granitic rocks is probably not a feasible task at the present time due to lack of data. It is expected that acquisition of reliable information will depend on sampling of test drillholes and investigations of the geochemical nature of fracture surfaces. Acquisition of undamaged fracture surfaces suitable for laboratory studies will probably be a very difficult task.

Prediction capabilities

We have indicated above that no results of any chemical analyses of groundwater from deep zones in plutonic rock mass of granitic composition were found in the literature. We will now consider the question of whether or not geochemical models exist that would enable the groundwater chemistry under these conditions to be predicted.

During the past three decades, thermodynamically based geochemical models for the prediction of groundwater chemistry have been developed to the stage of great power and elegance with regard to systems that proceed to thermodynamic equilibrium within the time-frame constraints of interest in some problems. In situations where many of the important reactions are very slow, equilibrium models based on thermodynamics can sometimes be used to define limits for water chemistry evolution. In other words, these models can sometimes be used to compute ranges of concentration values within which the actual water composition will likely occur. To do this however, it is necessary to be able to specify the mineral assemblage that the groundwater has come into contact with during its flow history, the order in which the various assemblages have been contacted, and the degrees of equilibration that have occurred along the various stages in the travel path - chemical evolution sequence. This type of approach to geochemical modelling of the pre-mining groundwater chemistry at proposed repository sites would probably yield useful information, but the level of uncertainty in the results will undoubtedly be very large. The uncertainties will accrue due to uncertainties in the thermodynamic data for the various minerals and aqueous dissolution products, and to uncertainties in the specific locations of travel paths that the water has followed prior to its arrival at the site of the proposed repository.

In addition to computational models that can be used to predict the evolution of the groundwater chemistry at various depths under various conditions of temperatures and pressure, there is a need for models that will calculate the dissolved species in the water based on chemical analyses from the laboratory experiments to determine retardation factors (distribution coefficients) for the various radionuclides in the fractured rock environment. With appropriate modification, the existing speciation models available from the U.S. Geological Survey (these models are known as WATEQ and SOLENEQ) should serve as a good base for calculation of the speciation of inorganic constituents in the natural groundwater. These models are now widely used for this purpose in groundwater investigations.

Evaluation of models

It would seem that model validation will have to rest primarily on the development of predictions for groundwater chemistry in sluggish flow zones in deep granitic rocks, followed by comparisons with results of chemical analyses of water samples collected from the zones for which the predictions are made. An appropriate starting point may be to compare model predictions with analyses of water samples from deep mine excavations or deep test boreholes. It should be kept in mind that the models must be tested against very old groundwater (i.e. thousands of years or more) in order to serve as a useful validation. The water samples to be used for comparison to model results must be proven to be old. It will therefore be necessary to conduct intensive isotope studies of the waters.

The modelling capability that currently exists for water-rock systems is almost entirely directed towards inorganic chemical interactions between water and its host rock. It must be kept in mind that the virgin groundwater in the repository zone will also contain small concentrations of dissolved organic substances. These substances are normally categorized as humic and fulvic acids (rather arbitrarily defined general categories that can include numerous specific organic molecules). These substances may cause mobilization of some radionuclide species to a level significantly beyond that which would be predicted from inorganic considerations alone. At present, there is little capability for predicting the effect on radionuclide mobility due to complexing with natural fulvic or humic substances. Some initial experiments by Cleveland and Rees (1976) suggest, however, that these substances have little effect on the mobility of plutionium and americium.

3.2.3 Geochemical conditions during the high-temperature period

During part or all of the period of groundwater inflow to the earth materials in the repository, the temperature of the rock mass near the repository will be much higher than is the case under natural conditions. Whether or not boiling conditions will occur will depend on the details of the repository design and spacing of spent fuel canisters.

In terms of long term migration of radionuclides from the repository towards the biosphere, the effect of elevated temperature in the rock mass may be important. Higher water temperature in the fractures will cause changes in the chemical interactions between the groundwater and the fracture surfaces. As a result, mineral precipitates (weathering products) or amorphous coatings on the fracture surfaces will undergo chemical and physical alterations. These changes may affect the permeability of the fracture networks. Of potentially more important consequence, however, would be changes in the retardation capabilities of the fracture surfaces. It is premature at this point to suggest whether the changes will increase or decrease the retardation capabilities. The important point is to consider the potential implications of these changes with respect to predictions of radionuclide transport in the fractured rock mass. If distribution coefficients determined by laboratory tests on chemically undisturbed fracture surface samples are used in simulation studies (presumably it will be several years before data of this type are available), large uncertainties may occur as a result of lack of knowledge of the effects of heat on the retardation capabilities of the fracture surfaces. If the zone of significantly elevated temperatures does not extend far from the repository walls, these uncertainties will be of little significance. If this zone extends upward into zones of more active long term groundwater flow, the uncertainties inherent in the retardation factors will be of great consequence.

We know of no way in which geochemical simulation models can be used effectively to provide estimates of the retardation capabilities of thermally unaltered fractured rocks. The predictive capability rests primarily on the acquisition of experimentally-determined distribution coefficients for the radionuclides of main interest. The question then arises as to whether or not geochemical simulation models can serve as a basis for prediction of the changes in retardation capabilities of the fractures as a result of elevated temperatures. In other words, given distribution coefficient values for the relevant radionuclides in aqueous solutions of specified chemical composition at normal groundwater temperatures, can the coefficients that are appropriate for use in zones that have been subjected to elevated temperatures be predicted within reasonable limits of certainty? The answer to this question remains to be established.

The question of whether or not uncertainties in distribution coefficient values in the zone of thermal alteration pose a significant problem in radionuclide transport rate analysis for the fractured rock zone between the repository and the biosphere,need not be pursued in great detail until after comprehensive analysis of the thermally induced flow conditions is completed. This analysis may demonstrate that the maximum zone of elevated groundwater and rock temperatures is limited to small distances from the repository walls. If this is the case, the thermal effects on distribution coefficients would be of little significance.

3.2.4 Geochemical conditions during the compressed air period

At some time after waste emplacement activities have ceased, it is expected that the shafts or tunnels that connect the repository to the ground surface will be permanently sealed. As indicated in section 3.2.3, the rock mass containing the repository will be relatively hot for several decades or more. Over the period of the temperature cycle, groundwater may flow into the emplaced earth materials in the repository. It is expected that the earth materials will have porosity in the range of about 10 to 25 percent. It is also expected that in their initial condition, the earth materials will be partly saturated with water. During the period of groundwater inflow, the water content of the earth materials will gradually increase until saturation is reached. Thus, air in the voids of the earth materials will be gradually replaced by water until the materials are saturated. The question of what will happen as air displacement occurs must be considered. The main gases in air are O_2 and N_2, with small percentages of CO_2 and other gases. Part of these gases in the air will dissolve in the water. Under conditions of normal atmospheric pressure, the amounts of these gases that will go into solution will be very small. As the process of air displacement continues, however, the remaining gas in the void spaces in the earth materials will be subjected to hydraulic pressures probably increasing to about 50 bars. As the total gas phase pressure increases, partial pressures of the individual gases will increase. Depending on the specific locations of the main zones of groundwater inflow, the gas phase in the partially saturated earth materials will be forced to new locations in response to the moving saturation fronts which are driven by strong hydraulic gradients. It is expected that gaseous zones under increasing gas pressure will form at various locations in the repository. As the partial pressures of O_2, N_2, CO_2 and other gases in the compressed air pockets increase, the amounts of these gases that will dissolve in the nearby pore water will also increase. Because of the increased dissolved oxygen, the pore waters in the earth materials will become strongly oxidizing. The increase in partial pressure of CO_2 will cause the pH of the water to decrease. In other words, acidity will be produced as a result of the increase in dissolved CO_2. If the earth materials have little buffering capacity, it is to be expected that the pH will greatly decline.

In addition to the acid-producing effect of increases in dissolved CO_2 caused by the pressurized air, acidity may be produced as a result of the large increase in dissolved oxygen that will result from air pressurization. From a geochemical viewpoint, the pore water in some or all of the earth environment in the tunnels will be strongly oxidizing. The dissolved oxygen content of aqueous solutions in contact with atmospheric gas (i.e. with oxygen at normal partial pressure of O_2) is about 8 to 10 mg/l (this depends to some extent on temperature). If the air in the voids of the earth materials is pressurized to several tens of bars, the dissolved O_2 concentrations in the pore water will be orders of magnitude higher than what is encountered in normal aerated waters.

An important consideration that must be addressed is whether or not the elevated dissolved oxygen concentrations will cause significant changes in the pore water chemistry. Of particular concern will be the evaluation of the effect of oxidation of small amounts of sulfide minerals (such as pyrite or marcasite). Oxidation of sulfur in these minerals to sulfate is one of the strongest acid-producing reactions known to occur in nature. If there are not sufficient quantities of acid-buffering minerals in the earth, the acid produced by sulfide oxidation will persist in the earth materials. If the acid is not neutralized, the situation may arise whereby some of the spent fuel canisters may come into contact with very acidic saline solutions. Depending on the composition of the protective material used to encapsulate the spent fuel rods, this may be a very undesirable situation. To insure that this possibility will not arise, there will be a need to design the earth containment system with the aid of hydrochemical simulation models.

Our evaluation of this problem has been limited to qualitative considerations. The most we can do in this brief review is attempt to identify the relevant processes that will occur during this period of compressed air formation. It appears that there is a possibility that the existence of zones of highly compressed air in the earth materials may cause the pore water in some tunnels or in parts of some tunnels to become highly oxidizing and acidic. This may occur during the high-temperature period, in which case steam production in the near-canister zone will further complicate the problem. These pore water solutions may cause the physical and geochemical nature of the earth materials to deteriorate significantly. The oxidizing, acidic pore water may occur near the spent fuel canisters. This may significantly affect the rate of dissolution or corrosion of the canisters. These pore waters may cause considerable reduction in the retardation capabilities of the earth materials in the repository, and may increase the hydraulic connectivity between the canisters and the surrounding rock mass.

It is evident that there is need for a detailed analyses of the repository environment during the compressed air period. This analysis must consider both the physical processes (two-phase flow) and the geochemical processes. In this situation, these processes are inseparable. The effect of the thermal regime is a further complicating factor.

If detailed analysis shows that there is a possibility that the acidity produced by gas compression will occur in significant amounts, it would be appropriate in the design of the earth materials to incorporate acid buffering materials such as calcite or dolomite. It may also be appropriate to include additives for control of the redox conditions. There may be a need, therefore, for development of an integrated physical-geochemical design of the earth materials. Emphasis must be placed on developing an earth system that will minimize the deleterious effects that will occur during the compressed air period, during the thermal period, and during the overlap segments of these two periods. Although these periods will not last long related to the full extent of the radionuclide activity, they may be extremely important with regard to the integrity of the overall containment system.

3.2.5 Diffusion of radionuclides through the earth materials

Since present plans for the repository design call for emplacement of clays and sands around the spent fuel canisters in the repository, it is of interest to consider the mechanisms by which radionuclides may migrate through these materials into the hydrological environment in the rock. If it can be shown that radionuclides will migrate into the groundwater regime in the rock within time periods that are short compared to the time necessary for decay to reduce activity levels to non-hazardous levels, then it may be necessary to place considerably more empahsis on studies of the groundwater regime than would otherwise be the case.

Regardless of whether or not they occur in simple ionic form or as charged or uncharged ligand complexes, radionuclides in water typically have molecular diffusion coefficients in the ranges of 1×10^{-5} cm^2/sec to 3×10^{-5} cm^2/sec. These coefficient values are appropriate for diffusion in aqueous solutions at $25^{o}C$. It is reasonable to expect that the diffusion coefficients for the radionuclides of interest are in this range, but little actual experimental data are available. The effect of temperature on the diffusion coefficients is probably relatively minor. The effects of diffusion resulting from a step-function input condition to a one-dimensional travel path have been computed using an anlytical solution of Fick´s second law of diffusion. The calculations indicate that over time periods as short as several hundred years, radionuclides at significant relative concentrations can migrate through many tens of meters of water. The use of coefficients for diffusion through water rather than through water saturated clay is of course a conservative approach. A more realistic approach is to base diffusion calculations on coefficients that are more appropriate for diffusion through saturated clay.

It is well known that diffusion occurs more slowly in saturated porous media than in aqueous systems in which there are no solid phase obstructions. This can be expressed by the relation between the diffusion coefficient for a solute species in water, D_W, and the coefficient for the same species in a saturated porous medium, D_p; viz.: $D_p = mD_W$, where $m < 1$. For dense saturated clays, m values are commonly in the range of 0, 05 to 0, 3. Thus, molecular diffusion in clay is somewhat slower than in free aqueous solutions. Calculations using diffusion coefficients in this range indicate that radionuclide fronts can diffuse through clay zones several meters thick in time periods as short as several hundred years. Therefore, if only several meters of clay separate the spent fuel canisters from the hydrological environment in the rock, it is possible that radionuclides will move into this environment long before radioactive decay reduces the activity to very low levels. In fact if the repository becomes saturated with water soon after the tunnels are filled with earth (i.e. within several decades), molecular diffusion is a process that may cause migration of some of the fission products through the clay into the rock system. It would appear that containment of fission products such as ^{90}Sr and ^{137}Cs, in the event that both the canister and retardation (adsorption and precipitation) are not entirely effective (this possibility is discussed in section 3.2.4), may not be achievable by means of compacted clay zones within the tunnels. If the probability of this situation is significant, then it would be evident that the only situation in which fission products such as ^{90}Sr and ^{137}Cs could be prevented from migrating into the rock system would be one in which the metallic claddings around the canisters remain completely intact for a period of time that exceeds the activity period of these nuclides.

The above mentioned diffusion calculations were made on the basis of relative radionuclide concentrations and an assumed step-function initial condition for the relative dissolved radionuclide concentrations at the exterior of a canister. In other words, it was assumed that the canister suddenly begins to yield radionuclides to the pore water in the porous medium around the canister. This initial condition is, of course, not realistic. Nevertheless, the calculations indicate that diffusion is a process that warrants further consideration in the development and evaluation of designs for emplacement of earth within the tunnels. Of particular importance in future model studies of the diffusive processes will be incorporation of more realistic information on the concentration-time relations for radionuclide emissions from the canisters. In other words, the rate at which the spent fuel matrix will dissolve after the metallic cladding losses its integrity is an important boundary condition in diffusion modelling. If the dissolution rate is extremely slow, the diffusive flux of radionuclides through the earth materials will necessarily be extremely slow. Also required for reliable modelling are radionuclide diffusion coefficients of the various radionuclide species. Based on analogy with data reported in the literature on experimental investigations of diffusion or inorganic solutes (ions such as Cl^{-}, SC^{2-}, Ca^{++}, Na^{+}, etc.) through saturated clays, there is about one order of magnitude of uncertainty in the diffusion coefficients that could be used as model input. To reduce this uncertainty, it will be necessary to conduct laboratory studies using samples of the earth materials that are to be used in the repository.

Prediction capabilities

Mathematical models are vailable for calculation of transient rates of diffusion through porous geological materials. With little difficulty, these models provide for one- and two-dimensional analysis of the diffusion process. The main limitations in this type of analysis will be the uncertainty in the rate at which the mass of spent fuel will contribute radionuclides to the pore water around the canisters during the long period of dissolution following rupture of the cladding. Even with this uncertainty, however, models of diffusional migration of radionuclides through the earth materials in the tunnels should provide very useful information. A parametric analysis should serve to identify the major possibilities with regard to diffusional flux of radionuclides from the earth materials into the surrounding rock mass. This information will be necessary as input conditions for analysis of radionuclide transport in the groundwater flow system in the rock mass. In the earth materials, it would be appropriate for some conditions to incorporate the effect of hydraulic transport (convection) as well as diffusion. Available transport models enable this type of analysis to be conducted.

In simulation studies of the diffusional migration in the earth materials, there will be some uncertainty in the values of diffusion coefficients. A more comprehensive review of the literature may permit estimation of these coefficients within about half an order of magnitude. This will be sufficient for many aspects of the simulation studies. Laboratory studies of diffusion in earth materials of the type proposed for the repository will be necessary as a basis for a more refined simulation analysis.

3.2.6 Retardation of radionuclide diffusion fronts within the earth materials

Processes

In section 3.2.5, it was shown that even in the complete absence of hydraulic gradients in the compacted earth materials in the tunnels, molecular diffusion will cause radionuclides to migrate outward towards the rock. It was indicated by preliminary analysis based on a simplified one-dimensional model that this outward radionuclide migration will occur at an appreciable rate relative to the very long periods of time during which many of the fission products and actinide species will persist at significant activity levels.

The only mechanism by which the diffusive flux can be limited or contained is chemical retardation. Chemical retardaion can occur as a result of processes such as adsorption, ion exchange, precipitation or isomorphous substitution. These processes, if they occur, would cause the radionuclide migration front to be retarded relative to the migration rate that occurs under non-reactive conditions. Retardation occurs for some radionuclide species because these chemical processes cause some of the radionuclide mass to be transferred from the pore water to the solid phase (i.e. to the porous medium). In other words, reactive radionuclides are partitioned between the pore water and the porous medium. In its simplest form (i.e. equilibrium reversible linear partitioning), the results of the partitioning processes are expressed in terms of a parameter known as the distribution coefficient, K_d

$$K_d = \frac{\text{weight of radionuclide in the solid phase per unit weight of dry porous medium}}{\text{concentration of radionuclide in the pore water}}$$

The normal units for K_d are ml/gram. If the K_d for a particular radionuclide species is large, the radionuclide is essentially immobile even under the influence of molecular diffusion. If $K_d = 0$, there is no effect

of chemical reactions on the mobility of the radionuclide species. To achieve long term isolation (i.e. for hundreds of thousands of years or longer) of a radionuclide species within porous geological materials emplaced around waste canisters in a repository tunnel, it is necessary that the Kd for the species in the saturated porous media be large.
Whether or not there exist geologic materials with adequate properties to satisfy this condition for each of the hazardous radionuclides remains to be established.

Formation of mobile complexes

Almost all of the literature on distribution coefficients for radionuclides in porous geological materials, such as clay, silt, or sand, pertain to fission products such as ^{90}Sr, ^{137}Cs and ^{60}Co. There is very little information on the actinide species. The literature dealing with ^{90}Sr and ^{137}Cs indicates that these species normally are strongly retarded in clayey materials. In the case of the Swedish crystalline rock repository, however, this information may be very misleading. This statement is based on the fact that nearly all fission product distribution coefficients reported in the literature pertain to laboratory tests conducted using non-saline pore waters. It is expected, however, that the Swedish repository will be located in a zone of saline water. The question arises, therefore, as to whether or not saline conditions will decrease the retardation capability of the earth materials emplaced around the canisters. As a preliminary estimate, we suggest that this will be the case. This judgement is based on the fact that there is abundant data in the literature indicating that many cationic elements form uncharged and negatively charged dissolved species. This occurs because of complexing with ligands such as HCO_3^-, $CO_3^=$, $SO_4^=$ and Cl^-. It is known, for example, that under some oxidation-reduction conditions that can occur in natural waters, plutonium forms relatively significant complexes with $CO_3^=$, HCO_3^-, $SO_4^=$, and CL^- (Andelman and Rozzell, 1970; Cleveland, 1970). Some of the complexes are positively charged, some are negatively charged and some are uncharged. It is reasonable to expect that the positively charged species will be much more strongly adsorbed on earth materials than the negatively charged complexes. It is reasonable to expect that the negatively charged plutonium complexes will undergo very little retardation during their passage through earth materials. In laboratory investigation, it has been demonstrated that increased HCO_3^- concentrations can cause a three- to four-fold decrease in the adsorption of plutonium on silica surfaces (Andelman and Rozzell,1971). This decrease was attributed to the effect of the formation of negatively charged complexes with cartonate species. Although there is little doubt that radionuclides such as ^{90}Sr and Pu species will form ligand complexes, we have not yet attempted to compute the degree of complexing that would occur under various assumed conditions of groundwater chemistry and initial radionuclide conditions. This topic is discussed in the next section.

Predictive capabilities

For reliable prediction of radionculide retardation in earth materials in the repository, it will be necessary to have data from detailed laboratory studies. In the laboratory studies, the earth materials that are to be emplaced in the tunnels must be used in conjunction with experimental aqueous solutions that are representative of the groundwater that will invade the repository tunnels at some time after their closure. Recognizing that it may be several years before adequate experimental data are available, the question arises as to whether or not some useful predictions can be made much sooner. A reasonable approach in development of preliminary radionuclide retardation predictions could be based on the following assumptions: (1) cationic (i.e. positively charged) radionuclide species are very strongly adsorded on the earth materials, regardless of their form of occurrence (i.e. as free ions, hydrated ions, or ligand complexes); and, (2) anionic and neutral radionuclide species are very weakly adsorbed on the earth materials, regardless of their form of occurrence.

If these assumptions are used, the main problem in retardation predictions is prediction of the partitioning of each of the important radionuclides between cationic and anionic or netural dissolved species. In other words, it is necessary to be able to compute the speciation of the radionuclides in groundwater of various assumed compositions. As more information becomes available on the chemical composition of groundwaters in potential or proposed repository zones, the calculation results of partitioning of radionuclide species would become more site specific. The critical step, however, is to establish whether or not ligand complexing in saline waters can cause excessive amounts of the most important radionuclides to become mobile in earth materials. In other words, given a specified rate of leaching of radionuclides from ruptured spent fuel canisters, the problem becomes one of computing the percent of each radionuclide that will occur as mobile species (anionic or neutral complexes). The availability of appropriate thermodynamic data will determine whether or not immobilization due to precipitation of solid phases can be included in the computational routines. The computations can be made using modified versions of existing inorganic aqueous-solution speciation models. The reliability of the computed speciation results will depend on the avilability of appropriate thermodynamic data for calculation of stability constants for the various complexes. It is expected that for some nuclides, existing data will be adequate and that for other species significant inconsistencies will arise. In some cases, re-evaluation of existing experimental data will be required.

3.2.7 Long term diffusion of radionuclides through rock fractures

In the event that radionuclides are leached from the canisters and migrate through the earth materials into fractures in the surrounding rock mass, the processes that would cause transport of the radionuclides towards the biosphere are: (1) advection (i.e. transport due to bulk movement of the water); (2) mechanical dispersion; and (3) molecular diffusion. As indicated in section 3.1.5, mechanical dispersion is not significant in groundwater regimes in which the velocities are very small relative to the diffusion rate. Under the best of circumstances, groundwater velocities in the fracture network near the repository will be sufficiently low such that diffusion could be taken as the dominant transport process. As indicated in section 3.2.5, molecular diffusion is a thermo-kinetic process that cannot be avoided, but which can be retarded if liquid to solid phase partitioning reactions are effective.

In this section, we will briefly examine the possible significance of diffusion as a mechanism for radionuclide migration through the fractures in the rock. Using the one-dimensional analytical solution for Fick´s second law of diffusion with a step-function input, it can be shown that, in the event of canister leakage, diffusion may cause migration of non-retarded radionuclide fronts at significant concentration levels. These fronts may migrate over distances of more than hundred meters from a canister in a period of 10000 years after initiation of leaching. If the repository facility is situated at a depth of 500 meters, the migration distances may be sufficient for entry of radionuclides into a zone of active groundwater flow. The zone of active groundwater flow could be a shallow zone of flow regime in a fault or shear zone located laterally from the repository. The diffusion analysis, upon which this statement is based, utilized diffusion coefficients that are typical of electrolyte species in water. In other words, the diffusion coefficients were not reduced by a tortuosity factor. It was assumed that the decrease in diffusion rates caused by whatever tortuosity exists in fracture aperatures is not very significant. At most, it would reduce the diffusion coefficients by a factor of only about two or three.

The results indicate that if radionuclides at appreciable concentrations enter the pore waters in the earth materials around the canisters during the first few thousand years of their existence, molecular diffusion may cause them to escape from the immediate vicintiy of the repository. This will occur if there exist interconnected fractures through which diffusion can take place, and if chemical retardation does not greatly retard the advance of the diffusion front. The main point we wish to make here is that a repository site in which the groundwater flow rates are extremely small does not establish a priori that radionuclide emissions to the biosphere will not occur.

In evaluation of the potential flux of radionuclides from the repository to the biosphere by molecular diffusion in non-advective groundwater systems, it will be necessary to have estimates of: (1) the possible rates of dissolution of the spent fuel masses; (2) the retardation capacity (i.e. distribution coefficients) of the fracture surfaces; and (3) the aperature widths and frequencies of the fractures in the zone between the repository and the shallow active groundwater zone. It is possible that detailed simulation studies of the diffusion process may establish that the flux into the biosphere would be insignificant. At present, however, it must be concluded that molecular diffusion in the rock must be viewed as a potentially important process. This will remain the case until it is proven otherwise.

If the repository is located in a zone of saline groundwater, diffusion may take on much greater significance than would otherwise be the case. This statement is based on the knowledge that some radionuclides such as strontium, plutonium, and americium are known to form mobile ligand complexes in saline solutions. Some of these complexes may undergo very little adsorption. This topic is discussed in section 3.2.8.

3.2.8 Retardation of radionuclides during migration through rock fractures

Processes

Based on the present state of knowledge, it can be assumed that radionuclides in the spent fuel canisters will eventually be leached into groundwater surrounding the wastes. Under the best of conditions, this will occur extremely slowly. It has been indicated in section 3.2.5 that chemical diffusion may cause migration of some radionuclide species through the earth materials into the rock. The question of potential travel paths and radionuclide migration rates in the rock system beyond the earth materials in the tunnels must therefore be addressed. If the groundwater velocities in the microfracture systems are very low, the radionuclides will migrate towards the biosphere (and in other directions) as a result of the chemical-kinetic process known as molecular diffusion. This process causes dissolved constituents to migrate in the direction of decreasing concentration gradients. Molecular diffusion occurs in the absence of advection or convection velocities, and of course can occur in the precence of advection or convection velocities in the bulk fluid mass in the fracture systems. Under the best of conditions, molecular diffusion will be the dominant readionuclide transport process. Under the worst conditions, advective or convective groundwater velocities will be the dominant mechanism of radionuclide transport towards the biosphere.

Chemical retardation is a general term used to describe the processes by which chemical reactions cause solutes (in this case dissolved radionuclides) to migrate such that the contaminant front travels more slowly than the bulk mass of the water. Chemical retardation slows down the migration for rates of contaminant fronts moving under the influence of molecular diffusion or under the influence of both diffusion and bulk fluid mass transport (i.e. advective and/or convective generated velocities). Chemical retardation is an important mechanism in radioactive waste management because it provides for larger decay periods along the pathway from the waste emplacement zone to the biosphere. Chemical retardation can occur due to ion-exchange reactions, adsorption reactions, isomorphous substitution, co-precipitation and precipitation. In other words, any chemical process that causes radionuclides to be transferred from the aqueous solution (i.e. from groundwater) to the solid phase (i.e. to the rock surface along the fractures) causes retardation. If the transfer is irreversible, then the radionuclides are permanently lost from the transport system. If the processes are reversible, then eventually, the radionuclides will re-enter the aqueous phase, except for those quantities that are lost by radioactive decay. Re-entry will occur when the water moving through the fracture system declines in concentration with respect to the radionuclide species under consideration. The process by which radionuclides are transferred by the above-mentioned reactions from the liquid to the solid phase can be referred to as liquid-to-solid phase partititoning, hereafter designated as LSP. The degree to which LSP occurs depends on the radionuclide species in question, on the physiochemical nature of the fracture surface, on the volume to surface area of the fracture, and on the temperature and chemistry of the fluid in which the radionuclide exists.

Prediction parameters

In order to evaluate the extent to which chemical partitioning will produce radionuclide retardation in a proposed repository environment, it will be necessary to know the LSP functions for each radionuclide species of interest in the groundwater of known composition in the individual fracture networks. In radionuclide transport studies, LSP functions are usually expressed as distribution functions or distribution coefficients, which express, for specified experimental conditions, the ratio of the amount of radionuclide that has been transferred to the solid phase to the concentration of the radionuclide in solution. Since these functions or coefficients are determined experimentally during a finite time period, they only represent the degree of partitioning that takes place during this time period. The value obtained therefore represents the results of the transfer reactions that occur relatively quickly. In the field situation, much longer periods of time will be available for the partitioning to occur. The experimentally-determined values from a reaction time viewpoint, therefore represent a minimum partitioning value. The approach whereby partitioning between liquid and solid phases is determined in the laboratory is often referred to as the "isotherm" approach. The "isotherm" is the relation obtained by plotting the amount of radionuclide on the solid phase (regardless of the specific transfer mechanism) per unit weight or surface area of solid phase <u>versus</u> the concentration of radionuclide that remains in solution after the partitioning has taken place. If the partitioning experiment is run at various radionuclide concentrations, a functional relation is obtained between the amount on the solid phase and the concentration in solution at various solution concentrations. This relation for the specified experimental conditions is known as the isotherm or as the distribution function. If this function is linear, it is known as a distribution coefficient. The distribution coefficient for granular materials is normally designated as K_d and is expressed per unit dry weight of porous medium. For fracture flow conditions it is designated as K_a and is expressed per unit area of fracture surface. If the isotherm is linear and if the effects of mechanical dispersion and molecular diffusion are neglected, a retardation factor for transport through fractures can be defined as:

$$V_w/V_p = 1 + K_a R_f$$

where V_w is the bulk velocity of the water that is transporting the radionuclide, V_p is the migration rate of the radionuclide front, K_a is the distribution coefficient expressed in units of L^3/L^2 (i.e. ml/cm^2), and R_f is the surface area to void space volume ratio for the fracture. If the isotherm is non-linear, this retardation relation is invalid. Nevertheless, it serves to illustrate the importance of retardation as a containment mechanism.

In the most simple terms, the problem of developing retardation predictions involves acquisition of data on K_a and R_f. In this section we will focus on K_a.

Prediction capabilities

From a retardation viewpoint, each radionuclide species should be considered individually. Each species has its own isotherm or distribution coefficient (K_a) for the specific condition under consideration. With regard to spent fuel the radionuclide species of main concern are the fission products; i.e., ^{90}Sr, ^{137}Cs, and the isotopes of the main transuranic elements, plutonium, americium and curium.

To our knowledge, there have been no K_a values (or distribution functions) reported in the literature for experimental conditions under which these nuclides, whether in combination or individually, have been passed in aqueous solutions through fractured granitic rocks. In fact, the deficiency of knowledge is such that there is hardly any information on K_a values for any type of fractured geologic material. With regard to fission products such as ^{90}Sr and ^{137}Cs, there is an abundance of experimental data for non-saline aqueous solutions in unconsolidated geologic materials and crushed (i.e. mechanically produced granular media derived from rocks) rocks. This type of data, when converted to a surface area basis from a per unit weight basis, indicates that it is reasonable to expect that under some conditions radionuclides such as ^{90}Sr and ^{137}Cs will be strongly adsorbed during passage through fractures in granitic rocks. However, since there are many factors that influence adsorption on rocks surface and since saline water conditions cause complexities beyond those that are typical for more simple aqueous systems, there is no firm basis at present for developing predictions of radionuclide retardation predictions in fractured rock systems of the type that may occur at potential Swedish spent fuel repository sites. Because values of K_a are not available for these conditions, inclusion of retardation terms in radionuclide transport models for the rock system cannot be expected to lead to very useful results. Unfortunately, there is no reliable basis for making even very general estimates of K_a values for fracture systems in granitic rock. Until this situation is rectified, all analyses of the consequences of migration of radionuclides from the earth materials into the rock system will contain large uncertainties.

Recent experiments at Argonne National Laboratory (Fried, et.al., 1976) suggest that plutonium and americium may be very strongly adsorbed in fracture networks. However, in these experiments, tuffaceous rock specimens were used rather than granitic rocks. The experiments were relatively crude. The effects of ligand complexing and redox conditions were not evaluated. It is doubtful whether the results can be transferred on even a qualitative basis to the problem of plutionium and americium migration through fractured granite in saline water. If an intensive research effort is mounted for evaluation of retardation (i.e. distribution coefficients) of the important radionuclides in fractured granite, relatively conclusive results may become available. At present there is not an established methodology for conducting reliable tests for distribution coefficients for fractured rocks. With very few exceptions, the literature on distribution coefficients in geologic materials pertains to the much simpler problem, that of determining distribution coefficients for non-saline solutions in non-fractured porous materials.

3.3 Heat transfer

3.3.1 Geothermal regime and thermal properties of the rock mass

Prior to the initiation of detailed thermal, hydrogeological or rock mechanics analysis of a conceptual repository design for short- and long-term containment, the in situ geothermal regime and rock mass material proterties must be identified and quantified.

The geothermal regime of any proposed repository site must usually be determined by field techniques. The same is true for the rock mass material properties. However, since this is usually difficult and always expensive, certain procedures can be utlizied to obtain approximations to the in situ states and properties. With these approximate methods, bounds on both the geothermal regime and rock mass properties can usually be obtained. Once the bounds have been established, the sensitivity of the repository design parameters to the range of the aforementioned variables may be assessed. This assessment subsequently allows a qualitative and quantitative realization of areas or properties which must be more clearly delineated through field exploration in order to have a high degree of confidence in the repository design.

As regards the geothermal regime prior to excavation, the most important variables which must be established are the temperature gradient, and the degree of nonlinearity in the temperature gradient, as a function of depth. The temperature gradient plays a significant role in determining when the heat from the radioactive waste starts to transgress in the downward direction. When heat is not flowing in the downward direction, all heat loss occurs in the horizontal and vertical directions with the most significant loss occurring vertically.

As an initial approximation to the temperature gradient, values in the literature can be utlized to determine tentative bounds on input to the conceptual repository design analyses (Clark, 1966). As stated previously, these bounds can then be utilized to assess the sensitivity of the thermal, hydrogeological and rock mechanics analyses.

The in situ mechanical and thermal properties of a rock mass are rarely obtained directly (Jaeger and Cook, 1969). Rather, laboratory measurements are generally performed on small samples of the rock mass taken from rock core, outcroppings or excavated rock. The laboratory properties are then utilized to extrapolate to the in situ properties through such considerations as sample size and frequency of discontinuities. The validity of this methodology is questioned by some, but the alternatives are highly impractical and expensive.

A considerable amount of mechanical and thermal properties of granitic rocks are available in the literature for room temperature conditions (Clark, 1966; Pine, R.J., 1976). The range of material properties generally available for granitic rock is presented in Table 3-1. This table is not intended to represent a composite of all the available information, but is merely provided to inform the reader of the approximate range of properties. The thermal conductivity of granitic rock is a function of homogeneity, discontinuities, water content, temperature and pressure. There presently are ongoing studies in the United States and Canada to assess the thermal properties of granites as a function of several of the previous variables.

A significant variable, which gives rise to the variance in the thermal conductivity of granitic rock, is the rock composition and crystal structure. A correlation between quartz content and thermal conductivity has been identified by Birch and Clark (1940). These investigations also found that, similar to other rocks, the thermal conductivity decreased with increasing temperature. In addition to the measurements made on relatively homogeneous granites, Assad (1955) has developed an equation for estimating thermal conductivity of fluid bearing, porous rock as a function of the thermal conductivity of the fluid saturating the pores and the porosity, viz:

TABLE 3-1

THERMO-MECHANICAL PROPERTIES OF GRANITIC ROCK

Property	Imperial Units	SI Units
Young's Modulus (E)	2 - 12 (10^6 psi)	1.4 - 8.4 (10^4 - MPa)
Poisson's Ratio (ν)	0.2 - 0.39	0.2 - 0.39
Unconfined Compressive Strength (C_o)	6, 000 - 47, 000 (psi)	41 - 324 (MPa)
Tensile Strength (T_o)	400 - 2464 (psi)	2.8 - 17 (MPa)
Density (p)	157 - 175 (lb/ft^3)	2.52 - 2.81 ($10^3 Kg/m^3$)
Thermal Conductivity (K)	0.9 - 3.6 (Btu/hr-ft-°F)	1.6 - 6.3 (W/m °K)
Thermal Diffusivity (a)	33 - 52 ($10^{-3} ft^2/hr$)	8.4 - 13.5 (10^{-7} m^2/sec)

$$K/K_1 = (K_2/K_1)^m$$

where: K = thermal conductivity of fluid saturated rock

K_1 = thermal conductivity of rock solids

K_2 = thermal conductivity of the fluid

m = an empirical exponent = $C\phi$

where C is a correlation factor ($\hat{=}$ 1.0)

ϕ is fractional porosity

The material properties of granitic rock at high temperatures have not been fully assessed; however, one can state that in general an increase in temperature lowers the rock strength and increases the ducility and deformational tendencey of rock. The mechanical behavior of discontinuities in granites subjected to elevated temperatures is even less understood. The degree of complexity in assessing thermal/mechanical discontinuity behavior and properties is much more difficult than that for homogeneous rock. However, rational bounds on granitic properties and granitic discontinuity properties can be hypothesized in order to assess the sensitivity of the repository design to variations in rock properties.

Consideration must be given to optimum waste emplacement conditions, in the sense of evaluating the maximum permissible thermal loading over the gross area of the repository facility. Based on the work of Cheverton and Turner (1972) for bedded salt in the U.S.A. as a guideline, one would conduct a parametric study of the induced global transient temperature field in the rock mass surrounding the waste emplacement, in which storage room geometry and rock behaviour, waste canister array and spacing, waste age and thermal power per canister are variables. The geological characteristics and thermal/mechanical properties of the site rock mass would be prescribed input. For the work conducted by Cheverton and Turner (1972), the following criteria had to be satisfied:

(1) maximum permissible temperature of the solidified waste;

(2) maximum permissible temperatures in zones surrounding the waste canister, as related to the deformational and failure characteristics of the rock;

(3) maximum permissible temperature rises at the surface and at specified near surface depths (say 30 and 100 m), and at the edge of a controlled buffer zone in the rock mass surrounding the repository facility.

For the current situation, involving a proposed repository facility in a granite rock mass, item (2) must be viewed in the context of fracture zone development and failure of jount planes. Item (3) is concerned with the influence of temperature on the groundwater motion and flow in aquifers. An additional criterion may be established in the sense of a permissible pertubation of the groundwater flow characteristics and the influx into or efflux of water from the waste emplacement zone of the repository.

3.3.2. Short-term rock mass behavior

The short-term thermomechanical response of the rock mass will by necessity be concentrated in the near vicinity of the emplaced radioactive waste packages. The response of the rock mass will be dependent upon temperature magnitude, temperature gradients, local hydrology, and post-mining stress states. Perhaps, the most significant of these variables is the temperature magnitude, since the pressure exerted by the fluid in the rock discontinuities will be greatly influenced by the temperture level. In fact, it has been hypothesized by some investigators that certain temperature levels might possibly induce local hydrofracturing in the repository, thus reducing the mechanical stiffness provided by the repository structurals. In this regard, significant effort should be expended in analyzing the temperature history of the repository environment in order ro identify engineering efforts which can reduce the repository temperatures.

A signigicant amount of approximate repository temperature histories is given in the literature (Schneider and Platt, 1974; Callahan, et.al. 1975; Cheverton and Turner, 1972; Ratigan, et.al., 1976).

These results have been developed through the utilization of both numerical methods and analytical solutions. The majority of the repository thermal analyses to date has been concerned with providing so-called worst cases to the rock mechanics investigations. The lack of repository ventilation has been assumed to provide the worst cases from a thermal/mechanical standpoint, and thus mine ventilation has generally been disregarded in most investigations.

Figure 3-2 displays the significance of repository ventilation. The results presented in the figure were obtained by introducing a plane radiogenic heat source (repository) in an infinite medium (rock mass) and subsequently superposing an additional plane which obeys Newton's law of cooling (repository ventilation). The results are for the repository plane and are presented as non-dimensional temperature versus non-dimensional time with the Nusselt number as the parameter which varies for each of the curves presented.

The temperature θ is non-dimensionalized with

$$\theta = \frac{2KT}{Q} \sqrt{\frac{\lambda}{\alpha}}$$

where Q = initial heat generation per unit area

K = thermal conductivity

α = thermal diffusity

$\lambda = -\ln(1/2)/\text{waste half life} = 0.693/\text{waste half life}$

Time is nondimensionalized with the decay constant λ. The repository ventilation is assumed to be sufficient such that a near constant air temperature is maintained. The figure indicates that the repository average temperatures are significantly reduced for nominal values of the Nusselt number. The average value of the Nusselt number for granitic rock can be expected to be in the range of 5 to 50, thus indicating a reduction of at least 60% in the average repository temperature through the addition of ventilation.

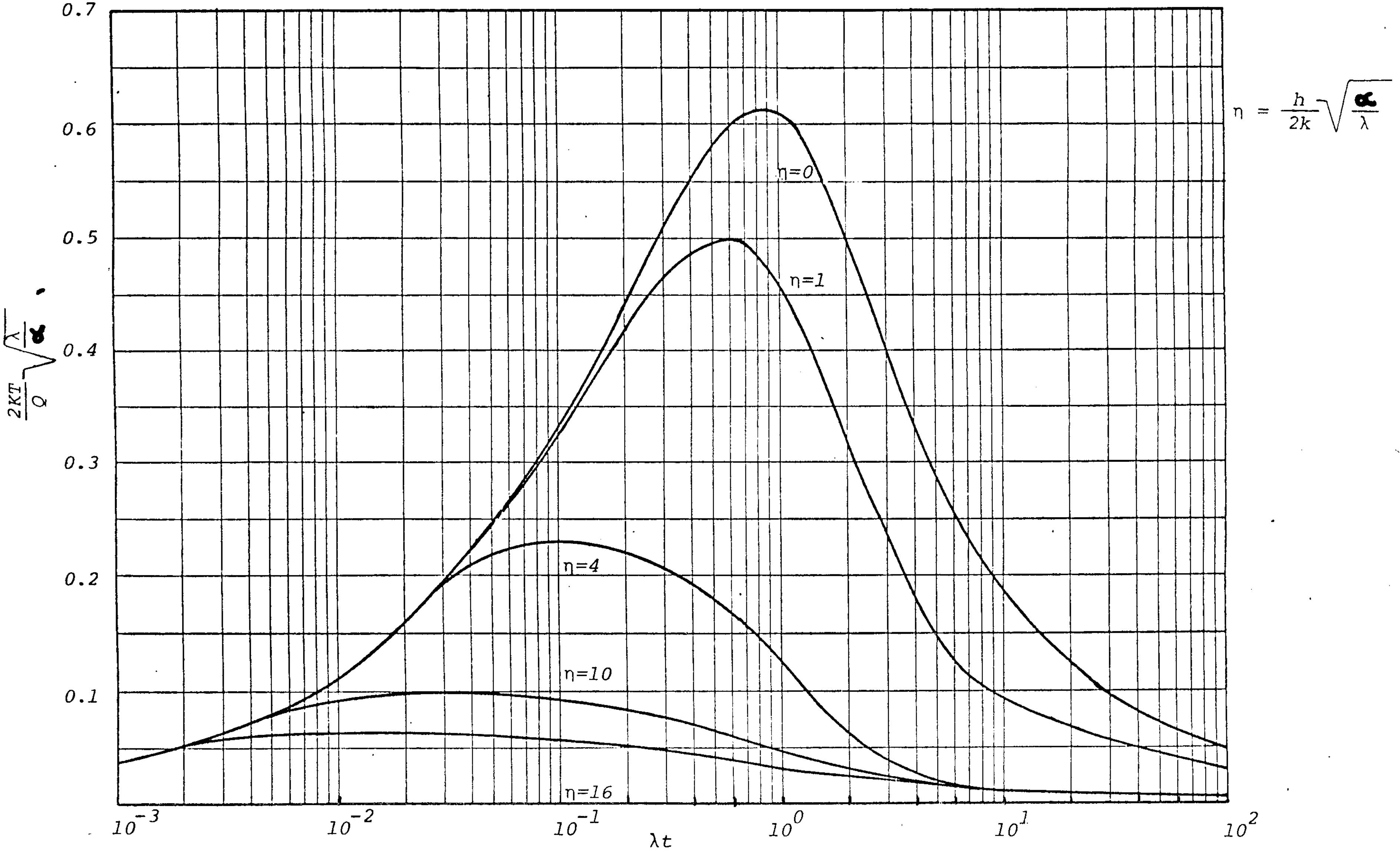


Figure 3-2. Average Repository Plane Temperature as a Function of Time and Nusselt Number

Whereas simplistic analyses, such as that previously described, can provide a quantitative notion of the repository temperatures and subsequent thermomechanical rock damage, the actual determination of what mechanical and hydrological events occur at a given temperature is a necessity. From the standpoint of waste package retrievability and waste packaging integrity, the local rock mechanics must be analysed. Thermal spalling of the rock on the drillhole periphery may negate the possibility of systematic waste canister retrievability, or may result in packaging failure leading to the possible introduction of actinides into the hydrogeological environment.

As evidenced by the quantity of temperature histories presented in the literature, the methodology for predicting repository temperature histories is well within the state-of-the-art for uncoupled thermal response. Numerical methods may be utilized to incorporate material and geometric non-linearities and inhomogeneous and anisotropic mediums. Analyses of hydrologically, mechanically and thermally coupled phenomena is not as easily performed.

Studies to assess the predictive capability of the numerical methods for temperature history calculation are presently being conducted in the United States under the direction of the Office of Waste Isolation, ERDA. The numerical methods are being utilized to predict the temperature history observed during the Project Salt Vault experiment conducted by the Oak Ridge National Laboratory (1971). Preliminary results indicate very good agreement between calculated and measured temperatures (Ratigan, 1976). Further verification studies are presently being planned in the United States as well as in Canada and Europe (Proc. Int. Symp. on the Management of Wastes from the LWR Fuel Cycle, 1976).

Monitoring of the waste respository radioactive levels, temperatures, deformations, hydrological behavior and stress levels is imperative in assessing long-term retrievability, the adequacy of sealing, and the potential for safe decommissioning. Monitoring during the operational phase of the repository will be of a greater magnitude than the monitoring occurring after waste emplacement due to the presence of mining and waste emplacement personnel.

Monitoring instrumentation sufficient for the operational period of the repository is presently available. Much of this same instrumentation is assumed to be adequate for the long-term monitoring of the repository, but again has yet to be demonstrated for long periods of time.

3.3.3. Long-term rock mass response

Prediction of long-term repository and rock mass response to the presense of radiogenic heat generation is the most important aspect of repository design and is undoubtedly the most difficult to perform and verify. Testing of rock and rock discontinuity response to load and temperature cannot be performed to represent the total time that must be utilized in the analysis of the repository. Rather, constitutive relationships must be extrapolated through orders of magnitude of time greater than that which occurred during laboratory or in situ testing. Verification of predictions of long-term behavior cannot explicitly be performed for obvious reasons.

The temperature history and resulting thermal cycle that a rock mass containing a repository will experience os highly dependent upon the type of radioactive waste which is resident in the excavation. Emplaced reprocessed waste, which is of the order of 10 years old, will result in rock mass maximum temperatures occurring on the order of less than 100 years for most of the rock. However, emplaced irradiated fuel (unreprocessed waste) results in a significantly different thermal cycle. In particular, a greater percentage of the entire rock mass experiences an elevated temperature environment due to the greater quantity of energy that is present in the unreprocessed waste. Presently, studies are being conducted in the United States and Canada to access the differences resulting from the emplacement of one or the other types of waste. The studies in the United States will concentrate on the prediction of maximum ground surface uplift and the potential for induced fractures.

Long-term monitoring will probably be performed on the surface or from subsurface facilities which have remote access to the repository environment. The long-term instrumentation should be designed to perform monitoring of:

(1) Vertical and lateral movement of the surface;
(2) Temperature of the subsurface environment;
(3) Level of radioactivity in the hydrological environment;
(4) Gross flow paths of the subsurface groundwater.

Vertical and lateral movement of the ground surface can be monitored directly or indirectly. This movement will occur due to subsidence, gross thermal uplift of the rock mass and gross tectonic activity. Measurement of surface movement is relatively easy to perform and can be rapidly evaluated. Temperature measurements will in all probability need to be performed at a considerable depth below the earth's surface. Temperature rises on the earth's surface will probably be shadowed by the seasonal variations in the thermal environment. A series of drillholes should be drilled in a region sufficiently large enough to incorporate the respository surface and the buffer zone for the temperature, radiological, and hydrological monitoring.

3.4 Rock mechanics

3.4.1. Scope of the rock mechanics aspect

From the viewpoint of rock mechanics modeling and the requirement of "a priori" facility design analysis for short- and long-term radioactive waste containment, one must have an adequate notion at the outset of the natural in situ state of stress, the requisite rock property parameters of the rock mass under consideration. Parametric studies may proceed on the basis of existing data for similar rock masses, but the results of such studies are primarily of value in bracketing design specifications. In order to address specific questions related to both short- and long-term containment, one must have specific quantitative data for a particular site to form a definite baseline from which the modeling efforts can proceed. The field equations which define the coupled behavior of a stress-temperature-flow situation in a rock mass are available from the fundamental laws of mechanics. For linear behaviour, without the inducement of rock fracture or flow, the appropriate material properties, can be utilized with the field equations to solve particular problems of a relatively idealized nature. For this situation, one would postulate linear rock deformation without limit, linear thermal behaviour, and a regular system of joints through which liquids would proceed under Darcy flow conditions. This type of analysis can proceed with minimal rock property information and hypothetical initial and boundary conditions. Due to the simplicity of the limiting assumptions, the results would be restrictive in application to practice, and could only serve to perhaps delineate the relative importance of various aspects of the coupled response in a hypothetical rock mass.

In actuality, the coupled rock response will be nonlinear, involving time-dependent deformation and fracture, temperature-dependent thermal properties, and stress-dependent flow conductivity in the joint systems and induced fracture zones. For this situation, one would postulate that the rock mass can be described as a nonhomogeneous continuum in the global sense, but must be considered a discontinuous media in the local sense. Specifically, when viewing the rock mass in a global sense, the flow conductivity of the in situ or pre-mining system of joints and their relative frequency can be thought of as being initially nonhomogeneous or "vertically stratified" from the surface to below the region of interest. The system of joints, or discontinuities, should exhibit rather regular spacing, allowing the entire rock mass to be described as a global continuum with a flow conductivity that is depth dependent (or initial stress dependent) and different in the horizontal and vertical directions (i.e., anisotropic). From a local viewpoint, on a scale that is comparable to the extent of the intended repository facility, the rock mass may be considered a discontinous medium, with homogeneous and anisotropic flow conductivities. Upon mining and emplacement of heat generating waste, which will give rise to stress and temperature perturbations, zones of induced fracturing will probably appear in the local sense about the repository facility and possibly in the rock mass above and below the facility in a global sense, depending upon the magnitude and dissipation of the thermal loading. In a global sense, the rock mass can still be viewed as a continuum with zonal definition of fracture zones that may grow with time. However, for analysis purposes, the flow conductivity of these zones may be regarded in the nonhomogeneous sense, similar to the initial vertical stratification for the undistrubed rock mass. The key element in the analysis is the global identification of these zones and the local quantitative evaluation of their flow properties. Locally, on the scale of the repository facility, the generation of fracture zones will be "quasi-static" in the short term due to stress gradients induced by mining and local heating, and of the creep rupture type in the long term due to stress gradients induced by transient thermal loading. The spatial extent and growth of the fracture zones will be influenced by the original system of joints, and to some degree by ventilation and back-filling of the repository facility. Almost certainly, the flow conductivity within the fracture zones and in the original joint systems will be dependent on the stress state, which will vary with time, and on the thermal driving force due to heat release from the emplaced waste.

From the viewpoint of rock mechanics analysis, both the global and the local approaches are necessary and interdependent. The basic field equations are effectively the same in both instances, but the constitutive relations are scale dependent. In the local sense, we must be concerned with both geometrical and material nonlinearities, and with discontinuous rock deformation such as occurs in fracturing processes. In the global sense, material nonlinearities are present, but discontinuous rock deformation may be "time-averaged" or assumed approximately continuous within the scales of time and spatial influence. Apart from field data for the state of in situ stress and the fracture and creep rupture characteristics for a specific rock mass, the analysis is conceptually tractable from a numerical viewpoint. The treatment of discontinuous rock deformation, such as occurs in fracture and creep rupture, and the corresponding growth of fracture zones in a time-space sense, are the weakest points. Clearly, these aspects are extremely important for quantitatively assessing flow conductivity and the likelihood of creating potential leakage paths. Formulations of constitutive relations for "quasi-static" fracture and creep rupture in a coupled stress-temperature-leakage paths. Formulations of constitutive relations for "quasistatic" fracture and creep rupture in a coupled stress-temperature-fluid flow environment are conceptually possible, but the current lack of laboratory data under controlled circumstances have limited the theoretical developments. The quantitative definition of the in situ state of stress, the regularity and extent of joint systems, and the nonhomogeneous and anisotropic flow conductivity for a given rock mass is possible, at least in an approximate sense, prior to mining. Obviously, these data would become better defined as a shaft is sunk and preliminary entries are developed in a selected site.

The following sections of this chapter will concentrate on the state-of-the-art of data availability, prediction and verification, and monitoring for the following four stages of a radioactive waste repository:

(1) Pre-mining
(2) Mining but pre-emplacement of radioactive waste
(3) Post-emplacement but short term in the sense of radioactive waste containment
(4) Long-term radioactive waste emplacement

No attempt is made to cite a large collection of related references, as the pertinent material has been published in many U.S., Canadian, and International symposia volumes and journals on rock mechanics over the past two decades. Rather, the intent is to scope the state of the art in a general sense as it may apply to the rock mechanics aspect of radioactive waste containment, and to identify key areas requiring further development and study.

3.4.2. Pre-mining

The pre-mining stage of a repository refers to the virgin or in situ state of the rock mass, prior to being disturbed by shaft sinking and entry excavation. Entry to the rock mass is achieved by drillholes, which should have very little if any perturbation on the global "undisturbed" nature of the rock mass. Apart from determinations of the in situ flow conductivity and thermal conductivity of the rock mass, which are treated in other chapters of this report, the principal items of interest for a rock mechanics analysis are:

(1) in situ state of stress;
(2) systems of joints, including spacing, orientation, and persistence with depth;
(3) elastic strength and fracture, and creep properties of the competent rock between joint planes, and of the rock in bulk including the strength and deformation characteristics of joint planes.

In situ state of stress

An assessment of the in situ stress field can be made by either theoretical considerations or field test procedures. From a theoretical point of view, the vertical in situ stress can be simply calculated on the basis of the weight of the overburden. By assuming a plane strain condition, the horizontal stresses will be equal to a fraction of the vertical stress, where the fraction is dependent on the Poisson's ratio of the rock mass. However, measurements of the horizontal stresses at depth in igneous rock have shown that the above calculation yields erroneous results; in fact, the horizontal stresses may not be equal and may vary from one to three times the value of the vertical stress. An alternate theoretical approach involves modelling, by the finite-element method, of the regional geological structure, including topographical irregularities. Since it is extremely difficult, and generally not realistically possible to model the time-wise formation of the rock mass and the assumed tectonic processes, this approach is currently more of academic interest than of practical value.

It is difficult and somewhat misleading to quote average in situ stress values which might be used for the conceptual design analysis, because the parameter is a function of the specific geological history, which is unique for each site. However, data published on stresses measured in situ do provide a broad range of values within which to work.

Field test procedures for the determination of the in situ stress field vary from hydro-fracturing of wellbores to measurements by strain relief techniques in drillholes in mine entries. Measurements by the latter techniques, including the borehole deformation gauge and the "doorstopper", in mines that are reasonable adjacent to an identified rock mass site could provide valuable and reasonably accurate information. The hydro-fracturing technique appears to yield reasonable results in situations where the vertical stress is in excess of the horizontal stresses. However, as the technique requires the generation of a crack in a plane normal to the least compressive stress, no useful quantitative information is obtained for the horizontal stresses when they are in excess of the vertical stress, as a horizontal crack is generated.

It is however quite evident, that none of the methods used to measure in situ stresses are free from objections. Partly, there are practical difficulties in making the measurements and partly, the results are to a large extent affected by residual stresses in the rock mass.

Joint systems and strength parameters

The identification of joint systems usually begins by surface mapping and proceeds with exploratory drilling, including the use of inclined drillholes. The use of a borehole camera or television, or a seisviewer, in deep holes, say to 1, 000 metres, is potentially feasible, but it is doubtful that such an application has been made to date. The recovery of oriented core from inclined drillholes should provide useful information on the spacing, orientation, and persistence of joint systems with depth.

The shear strength developed along the discontinuities is of great importance to the local and eventual stability of an underground excavation. The surfaces of the discontinuities may be smooth, or rough, undulating or planar and contain minerals as clay. These details all affect the shear strengths available to maintain the competency of separate blocks or zones adjacent to excavations. However, for preliminary desigh studies, precedent data are of great use in conjunction with the assumptions made for the joint set frequency and orientation. A useful summary of joint shear strenghts is provided by Barton (1972). From a statistical consideration of these data, the following relationship was proposed:

$$\tau/\sigma_n = \tan\left(A \log_{10} (C_o/\sigma_n) + 30^\circ\right) = \tan\phi^\circ$$

where τ = joint shear strength (MPa)

σ_n = joint normal stress (MPa)

A = constant as follows:

Rough, undulating joint surface: A = 20

Smooth, undulating joint surface: A = 10

Smooth, nearly planar joint surface: A = 5

C_o = unconfined compressive strength of adjacent rock (MPa)

However, nominal rock stresses in the vincinity of the proposed repository at a depth of 1, 000 metres may be in certain cases considerably higher than the normal stresses at which the data for the above values were obtained. This may cause a slight reduction in the available friction angle, but is not thought to be of major significance. In addition, a destressed zone (due to blasting) will probably extend up to 2 metres from the room wall, depending on the blasting techniques used, the type of rock, and the extraction ratio.

If the rock joints are filled with secondary minerals such as clays from hydrothermal alteration or rock gouge from joint movement, the available friction angles may be much lower. Within granite and gabbro rocks, these lower values might be of the order of 20 degrees or even less. The existence of such infilling materials may thus give rise to rock engineering problems within the immediate vicinity of the rooms where confining and normal stresses may be low. Therefore, careful site investigation is required to identify the frequency of occurence of clay or gouge filled joints, and rock masses having a predominance of these features should be excluded from consideration.

It is also quite clear that the factors which influence the unconfined compressive strength also influence the shear strength of the joint.

On analyzing the groundwater flow as related to problems of a rock mechanics nature, the normal and shear stiffnesses of the joints must be determined. Those properties vary according to the width of and normal stress across the joints. A systematic investigation of the stiffness existing for stresses at a depth of 1, 000 metres has not been done. For considerably lower normal stresses and for unfilled and very thin joints, values for normal rigidity are of the order of 200 MPa/cm and for shear stiffness of approximately 5-10 MPa/cm.

Fluid flow conductivity of joints

These discontinuities will dominate the ability of the rock mass to conduct water, since the permeability of the intact plutonic rock material itself is extremely low, decreasing with increasing confining pressure. Laboratory test results for rock core samples with artificial and natural fractures indicate that the flow conductivity of the fractures is substantially reduced for normal stresses in excess of 40 kg/cm^2 (Witherspoon and Gale, 1976).

For the purpose of estimating the flow rates that a systematically jointed rock mass can sustain, it is convenient, analytically, to treat the rock mass as a porous medium. For exampel, assuming a cubic arrangement of interconnecting joints (which has been observed in granite rock masses) of constant width, the permeability of the rock mass can be equated to the joint width and spacing by the following equation due to Snow (1972):

$$K = (b^3/12s) \times 10^{-7}$$

K = rock mass permeability (metres/sec)
b = joint width (metres)
s = joint spacing (metres)

Data have been obtained at depths to about 100 metres, where the opening of joints due to weathering may still be significant, with values varying between 10^{-9} and $30 \cdot 10^{-9}$ m/sec. At a depth of 1, 000 metres in a preselected competent plutonic rock mass, it can be expected, therefore, that the overall rock mass permeability due to systematic joints will be less than 10^{-9} m/sec and probably of the order of 10^{-10} m/sec. However, the permeability of a zone around an excavation will probably be greater than these values due to fractures created by blasting and stress gradients. Under these conditions, the achievement of inflow rates equivalent to overall mass permeabilities of the order of 10^{-8} m/sec and less, including systematic joints and singular features, will be determined by the effort involved in grouting the singular features. Using a combination of cement, bentonite and chemical grouts, recent work in Sweden has resulted in mass permeabilities of the order of 10^{-10} m/sec in previously permeable singular features in granite (Bergman, et. al., 1974).

Rock strength and deformational characteristics

The recovery of core from vertical drillholes would provide intact rock samples for laboratory determinations of elastic, strength and fracture, and creep properties. The elastic properties, i.e. Young's modulus of elasticity and Poisson's ratio, and the strength and fracture properties, including residual strength, can be accomplished without difficulty under uniaxial loading conditions. The evaluation of these properties under confinement stress is slightly more difficult, and becomes increasingly so when elevated temperature and fluid flow within the sample are introduced. The lack of available equipment to accomplish these latter tests on a production basis is of particular concern. The core obtained from inclined drillholes can be used to evaluate the strength and deformation characteristics of joints, assuming that the drillholes intersect joint systems.

Commonly, the results of triaxial compression experiments are represented by a sequence of stress circles on a Mohr diagram, to which a failure envelope may be fit. The failure envelope may be represented mathematically in terms of principal stresses and a failure parameter in the sense of a yield condition, similar to the procedures used in plasticity theory. If the granitic rock exhibits little or no plastic deformation at confining pressures and temperatures up to 300 kg/cm^2 and 200°C, respectively, then the failure condition represents a limiting condition for fracture. Data, as obtained in the laboratory under much higher confining pressures and temperatures on granitic rocks, indicate only modest plastic deformation with ductile fracturing at relatively small stresses of 10% (Handin, 1966). The residual strength of the fractured rock may be of the order of 20 to 25% of the intact rock strengths, and can be represented mathematically as a post-failure condition.

The strength of a rock is dependent upon the physical dimensions of the specimen, partly due to the microfractures and partly due to the techniques of data accumulation and reduction. In general, test results for uniaxial compression of rock specimens at room temperature indicate a reduction of up to 75% in compressive strength with increasing specimen dimensions in addition, test results have demonstrated a reduction of 20 to 40% in strength when the rock is saturated with water.

The modulus of elasticity of a relatively small laboratory rock specimen may be considerably greater than that of a large block of rock subjected to full scale loading. Once again, this discrepancy is partly due to microfractures and joints in the large block, and partly due to the methods of testing and data reduction.

The most difficult tasks in the determination of rock properties are those related to assessments of creep and creep rupture characteristics and of bulk (or macroscopic) in situ properties of all types, particularly under simulated conditions of confinement stress, elevated temperature, and fluid flow. For relatively short-term loadings under ambient temperature conditions, the creep deformation of a specimen of granite will be negligible. With elevated temperatures and sustained states of stress near the yield strength of the rock, the creep deformations over long periods of time may be significant, and may lead to creep rupture. Data for the long-term creep of granite is very limited, and the constitutive law formulation of such phenomena is quite primitive. Basically, the lack of available laboratory equipment and consistent formulations of appropriate constitutive laws are a severe hindrance to the evaluation of creep and creep rupture characteristics, even on a research scale. The determination of bulk in situ properties is essentially impossible by use of drillholes for the depths anticipated. Such properties must either be determined in adjacent mines or in the preliminary openings of the repository facility, and will be discussed in more detail in Section 3.4.3.

Some fundamental data from the literature are presented in Tables 3-1 and 3-2 for the elastic and strength properties of some igneous rock types. Generally, the data are rather inadequate, but ranges of values are indicated.

Relevance of data requirements

In order to assess the short- and long-term stabilities of a proposed repository facility, the above properties are necessary input to a representative form of stress analysis. Commonly, the analysis of the induced stresses, deformations, and rock fracture and/or creep rupture due to the mine excavation and subsequent thermal loading would proceed by some form of numerical analysis, such by the finite element or finite difference methods. Numerical solution procedures are required because of the complex geometries, local discontinuous nature of the rock mass, material nonlinearities, and coupled stress-temperature-fluid flow phenomena. Computer codes are available for treating certain coupled aspects of the situation, but are relatively scarce or nonexistent when such phenomena as post-fracture behaviour, joint systems, and creep rupture are introduced. Additional discussion of these facets of analysis will be given in subsequent sections of this chapter.

3.4.3. Mining/pre-emplacement

The mining/pre-emplacement stage of a repository refers to the underground construction or mining activities that precede the actual emplacement of waste. In particular, this would include shaft sinking, shaft station excavation, and the development of haulageways, ventilation drifts, and rooms for emplacement of waste. These mining activities will give rise to stress perturbations in the

Table 3-2

Strength Properties of Some Igneous Rock Types (Handin, 1966, pp. 273-274)

Rock	Unconfined compressive strength, C_o (MPa)		Cohesive strength S_o (MPa)	Angle of Internal friction		$\sigma_1 = A + B\sigma_3$		Tensile strength $T_o = -A/B$ (MPa)
	Average	Approx. range		ϕ (o)	Tan(ϕ)	A (MPa)	B	
Granodiorite (Australia)	126.9	66.9-186.8	17	56	1.5	111.0	10.7	10.3
Salt Lake (?) Hypersthene Andesite (Idaho/USA)	133.1	120.7-145.5	29	45	1.0	137.9	6.1	22.6
	128.9	116.9-141.0	28	45	1.0	131.0	5.7	23.0
Miocene Basalt (Oregon/USA)	168.9	153.1-185.1	32	50	1.2	170.0	7.4	23.0
	218.9	161.0-277.2	44	48	1.1	224.1	6.6	33.9
Quartz Diorite (Idaho/USA Batholith)	86.9	82.0- 92.0	14	54	1.4	85.2	9.2	9.2
Swandyke Diorite Gniess (Colorado/USA)	63.1		11	52	1.3	65.8	9.0	7.3
	104.1		18	54	1.4	111.0	10.0	11.1
Colville Granite (Wash./USA)	148.9	106.9-191.0	23	58	1.6	154.1	11.8	13.0
Altered Colville Granite (Wash./USA)	65.2	47.9- 82.0	10	58	1.6	66.9	11.9	5.7
Precambrian Granite (Colo./USA)	72.1	45.5- 98.6	14	56	1.5	92.0	11.1	8.3
Precambrian Pegmatite Granite (Colorado/USA)	42.1	26.9- 56.9	7	58	1.6	50.0	11.8	4.2
	57.9	57.6- 58.6	8	52	1.3	45.9	8.9	5.2
Monzonite Porphyry , Colville Batholith (Wash./USA)	124.8	86.2-163.4	17	60	1.7	120.0	13.4	9.0
	173.1	140.7-205.5	20	65	2.1	166.2	17.7	9.4
	170.0	93.4-246.5	22	56	1.5	141.0	10.3	13.7

peripheral regions of the openings, and a "local" alteration of the overall stress field in that portion of the rock mass which encompasses the repository excavation as a whole. For a granitic rock mass which is globally "stiff" as compared to say a salt formation, the deformations and zones of fracture generation around the openings should be small, say to a depth of at most 10% of the largest opening dimension, if the extraction ratio is relatively small as compared to conventional ore mining. Creep and "psuedo-plastic" flow of the igneous rock will be essentially non-measurable. The zones of local fracturing will be highly localized in the immediate periphery of an opening, and will be influenced to a certain extent by the spacing and strength of the joint planes. A regular system of rock bolting, with accompanying wire netting, would ensure competency of the ribs and roofs of the entries and emplacement rooms for common ambient working conditions.

For this stage of the repository facility, from the viewpoint of rock mechanics, one would concentrate on the following:

(1) determination of the in situ stress field;
(2) detailed mapping of the joint systems, including spacing, orientation, and regularity;
(3) measurement of the depth of the zones of induced fracturing around the openings;
(4) determination of in situ rock strength and deformation properties;
(5) sophisticated in situ heater tests for gauging rock response to the simulated emplacement of radioactive waste;
(6) continuation of laboratory tests on rock core from the immediate vicinity of the repository facility, for assessment of fracture and creep rupture characteristics under simulated stress-temperature-fluid flow conditions;
(7) emplacement of instrumentation for monitoring temperatures and rock stresses and deformations after waste emplacement.

The measurements of hydrogeological parameters, including water influx, are discussed in another section of this report. The field and laboratory data mentioned above would be used for short- and long-term stress analyses of the rock mass encompassing the repository facility, for both ambient and elevated temperature conditions.

In general, the purpose of gathering rock mechanics data in the mining/pre-emplacement stage of a repository is to refine the various aspects of the long-term containment analysis, and to make necessary changes if required in the facility design. Ideally, one would like to install instrumentation for monitoring long-term temperature, stress, and water migration fluctuations within the immediate vicinity of the repository.

In order to assess the in situ stress field, one would probably make use of one or more strain-relief techniques, such as the borehole deformation gauge, "doorstopper", or thin-walled vibrating-wire stressmeter. All three of these techniques utilize overcoring procedures, and the first two have been widely used with good success in igneous rock masses. These techniques become more difficult to use if the rock mass is highly jointed or fractured. In this instance, consideration would have to be given to the use of flatjacks in the periphery of an opening, or to a borehole jacking technique.

Assessments of the joint systems and the depths of fracture zones can be made from conventional coring techniques. Of all of the data to be gathered, these two items should present the least difficulty.

The in situ strength and deformation properties of the rock mass can be assessed by borehole jacking and flatjack tests (Patricio and Beus, 1976; Heuzé, 1976; Handy, et.al., 1976; Hustrulid, 1976). In particular, one wishes to evaluate the strength and deformational characteristics of a relatively large portion of the rock mass, as compared to a laboratory test on a small rock specimen, including the influence of the joint planes. The in -situ strength of the joint planes are also of interest. These tests are time consuming and occasionally difficult if the rock is badly fractured, but the results are invaluable and amenable to evaluation by numerical simulation procedures. In general, one would expect the "stiffness" of a jointed rock mass to be less than that of a small specimen. However, by properly modeling the jointed rock mass and utilizing the results of selected laboratory tests on small rock specimens, the "stiffness" of the rock mass can be calculated and compared with the in situ test results. Continuation of laboratory tests on small specimens of the site rock, say cylinders or cores with diameters of ten centimeters and lengths of twenty centimeters, is imperative. These tests should be conducted under specified conditions of applied stress, temperature, and fluid flow, in order to assess the quasi-static and creep rupture characteristics of the rock.

The design, installation, and operation of sophisticated heater experiments are absolutely necessary for assessing the "local" response of the host rock to the simulated emplacement of heat-generating waste (McClain and Bradshaw, 1971; Van Sambeek, 1976). If retrievability of waste is a requirement, then the heater elements would probably be encased in steel sleeves that are emplaced in vertical drillholes in the floor of a room. Apart from hydrogeological considerations of water influx to the heater emplacements, one would want to measure the induced temperature field and thermally-induced rock stress variations with time. The temperatures can be measured with conventional thermocouples encased in drillholes around a heater installation. The thermally-induced stress variations can be monitored with vibrating wire stressmeters emplaced in drillholes. In addition, borehole extensometers can be used to measure "internal" rock strains, and floor and roof pins to measure floor heave and roof-to-floor closure. In order to assess thermally-induced fracturing around the heater emplacements, one could perhaps periodically drill small holes and recover the core. The response of an emplaced vibrating wire stressmeter might also be used to gauge the growth of fracture zones, but this technique has not been evaluated or calibrated in the laboratory to date. These experiments provide an unique opportunity to evaluate the predictive capability of numerical modeling techniques, where in laboratory and in situ strength, deformation, and fracture data are utilized in the calculations.

The number of cases where rock mechanics response has been predicted by modeling procedures, such as by the finite-element or finite-difference methods, and verified by case history data, is relatively limited at the current time. The constraints are largely in the areas of realistic constitutive law development, economics of large two- and three-dimensional simulations, and lack of bonafide field data for comparative purposes. Recent efforts to simulate case history data from underground salt mines and the Project Salt Vault experiments have yielded very promising results (Bradshaw and McClain, 1971; Callahan, 1976; Hofmann, 1976; St. John and Hardy, 1976). The latter data represent an induced thermal loading situation in a bedded salt formation, as developed by carefully designed in situ heater experiments. Case history data for a composite stress-temperature-fluid flow situation are probably only available for hot-water flooding or steam injection of oil reservoir formations; these data would represent information gathered in a remote fashion from the actual formation being stimulated.

The instrumentation available for the long-term and perhaps remote monitoring of the repository facility is somewhat limited, and certainly has not been tested for periods of time much in excess of a decade. Thermocouples could be emplaced in the rock mass throughout the immediate repository facility for temperature measurements. Vibrating wire stressmeters, installed in drillholes, could be used for monitoring stress changes, but their long-term endurance is unknown. Roof-to-floor convergence and floor heave are relatively easy to measure by conventional surveying practices, but access to the emplacement rooms and the adjacent entries may be difficult after several decades. The monitoring of groundwater motion is possible by remotely placed drillholes, but may be difficult in the immediate area of the waste emplacements due to drillhole instability and collapse.

3.4.4. Post-emplacement/short term

The post-emplacement/short-term stage of the repository refers to the period of time from waste emplacement to 300 to 500 years after emplacement. During this time period, the repository facility will almost certainly be decommissioned and perhaps sealed, and the peak temperature rise in the rock mass encompassing the facility will have occurred. The thermal expansion and contraction of the rock mass in the global sense can be viewed as a surface uplift and gradual subsidence. In effect, the interior of the rock mass will be subjected to a "flexing" which may result in the growth of fracture and creep rupture zones in the near vicinity of the waste emplacement, and possibly to a limited extent in the far field. There are no data available as a case history for such a situation. The analysis must certainly proceed with a thermal analysis to evaluate the temperature history, followed by a thermostress analysis to evaluate the potential for the generation of fracture zones in the rock mass. The generation of fracture and creep rupture zones is effectively a process involving dilation, which should enhance the flow conductivity. Once the timewise growth of the fracture zones is identified, then the flow analysis can proceed. In the absence of fluid flow, the problem is coupled in a one-way fashion, in that temperature is effectively independent of stress level. With the introduction of a fluid, the fluid motion is dependent on the temperature history and on the growth and conductivity of fracture zones due to the induced thermal stresses. The rock stresses in the near field of the waste emplacement will probably be dependent on the fluid motion, particularly if the temperatures are near or above the boiling point of the water.

The computer codes to handle a stress-temperature-fluid flow problem in a coupled sense, including allowance for fracture zone growth, are not currently available. The growth of quasi-static fracture and/or creep rupture zones is a nonlinear situation, and the fluid conductivity in the zones will be both stress and temperature dependent. Due to the massive thermal expansion of the rock mass, the joint planes in the near and possibly far fields, outside the fracture zones, may open, depending upon their strength, and increase the global flow conductivity. At the current time, it would appear that the problem has to be partially uncoupled, within the capabilities of the individual available computer codes, and then recoupled in an iterative process in time. The constitutive laws for either quasi-static or creep fracture initiation and growth under coupled stress-temperature-fluid flow conditions are extremely primitive, due in part to the lack of experimental data. The prediction of flow conductivity for thermally induced fracture zones on a macroscopic scale, as well as for joint planes subjected to thermostress conditions, is certainly much more qualitative than quantitative. Field data are also extremely limited, as case histories analagous to the repository are certainly rare, if perhaps nonexistent.

The monitoring of the stress-temperature-fluid flow histories in the near and far fields to the repository will certainly be accomplished by remote techniques, based on the current state-of-the art, and will involve the use of instrumented drillholes. The drillholes may be subjected to collapse in the near field due to the potential growth of fracture zones, and to the relatively high states of thermal stress. Monitoring of the surface uplift and subsidence can be accomplished by precision surveying procedures.

3.4.5. Post-emplacement/long term

The post-emplacement/long-term stage of the repository refers to the period of time beginning some 300 to 500 years after emplacement and ending with the decay of the waste elements to a level that is harmless to the life environment. The peak temperature rise in the rock mass, as a consequence of the waste emplacement, has long since passed. The growth of fracture zones has terminated, and the entire rock mass begins to relax back toward its original state. The rock deformation is certainly of a creep nature, with consolidation of the fracture zones and "tightening" of the joint planes. The flow conductivity of the rock mass will be reduced, perhaps substantially as the temperature field returns to the geothermal equivalent. The processes of erosion, glacial loading, and crustal movements, in the long-term geological sense, may occur.

From the viewpoint of the rock mechanics analysis, which will involve long-term stress and deformation changes, one must consider three contributing factors; viz:

(1) the results of the analysis of the post-emplacement/short-term stage which form in effect the initial and boundary conditions to post-emplacement/long-term analysis;

(2) the extrapolation of laboratory and in situ results obtained under conditions of combined stress, temperature, and fluid flow, but over periods of years, to the analysis of phenomena involving hundreds and thousands of years;

(3) the introduction of long-term geological processes such as erosion, glacial loading, and crustal movements.

Assuming that the analysis procedures are capable of adequately evaluating the rock mechanics phenomena under the post-emplacement/short-term stage, then the analysis of this stage should certainly be no more difficult. Furthermore, the results of the short-term analysis should adequately provide the initial and boundary conditions at the outset of the long-term analysis. The difficulties arise in the use of laboratory data on rock behaviour for an analysis of phenomena that occur over many orders of magnitude of years, and in incorporating the likelihood of long-term geological processes and their relative magnitudes of disturbance. These considerations must certainly fall within the scope of an integrated risk and uncertainty analysis.

4. PROPOSED STUDY PLAN

4.1 General approach

The overall objective is to develop a description of the groundwater flow field in the repository region in order to provide the best possible data for saftey assessments. As discussed in section 2, the problem requires recognition of many simultaneous and long lasting complex processes.

We have developed a program in which the central effort is the development of simulation models for the significant processes in each of the principal repository phases. These include fluid flow, geochemical, heat transport and rock mechanics. In order to provide definition of the problem and produce input data, additional efforts are required on site geology and geotechnical parameters.

In order to assist in the interpretation and subsequent application of the results, we have outlined a limited effort on geochemical aspects and containment transport modelling.

The nature of the problem at this stage unavoidably involves the recognition of uncertainty in the description of the site and its hydrogeological properties. Furthermore, modelling of such a complex system involves major approximations in certain cases. We therefore propose to develop the simulations in a semi-probabilistic framework rather than simply to treat "best estimates" or "worst cases" in a piecemeal manner. We therefore intend to develop an overlay probability model to associate probability estimates with output results.

A number of elements to be studied and a proposed time schedule are given in Figure 4-1. The reporting from each study element is scheduled according to following table:

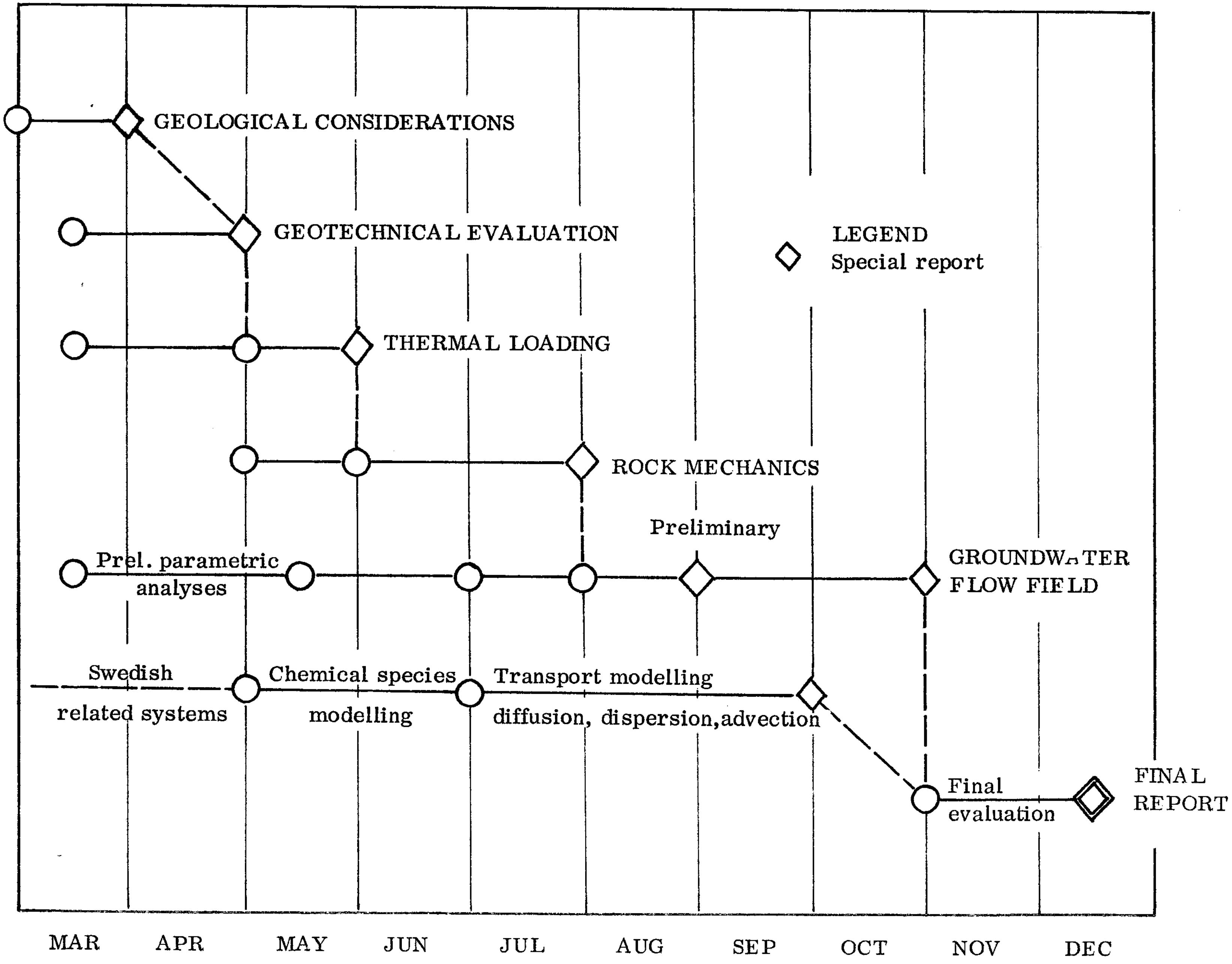


Figure 4-1. Study Elements and Time Schedule.

Study element	Start	Special report
Geological considerations	Mar 1	Apr 1
Geotechnical evaluation	Mar 15	May 1
Thermal loading	Mar 15	Jun 1
Rock mechanics	May 1	Aug 1
Groundwater flow field	Mar 15	Nov 1
Geochemical	May 1	Oct 1
Final Evaluation	Nov 1	Dec 15

The program objectives for various time stages of the repository are presented in Figure 4-2.

4.2. Geological considerations

Systems of joints, faults, shear or bedding planes which intersect the rock mass will be of critical importance to the hydrological conditions within the rock mass. A critical judgement of these factors is thus called for.

The objective of this first study is to provide relevant geological data from suggested repository sites in Sweden. With the background given in section 3 on the state of knowledge relevant to depths in excess of 500 meters in the Fennoscandian shield, it becomes clear that much of the data will have to be aquired through new investigations. A rather comprehensive geological investigation program (including seismology and hydrology) is being carried out in Sweden and the information will be used as input in this sudy. Furter exploratory field tests will also be suggested, if necessary.

Examples of projects which will be of great value to this project are the in-situ experiments in the Stripa mine and deep hole drilling at proposed repository sites.

	Virgin (Pre-Mining)	Construction (Pre-Emplacement)	Short Term Containment	Long Term Containment
FLUID FLOW	Development of regional flow model as reference state	Simulate effects of repository construction in near field	Simulate repository inflow and recharge and thermal response	Long term regional flow field and travel times
HEAT TRANSFER			Determine transient temperature field in rock mass due to waste emplacement	Evaluate long-term temperature changes and return to geothermal conditions
ROCK MECHANICS		Evaluate stress and displacement fields due to mining excavation	Determine stress and displacement response due to temperature field and evaluate fractured regions	Determine stress and displacement response due to temperature decline and consolidation of fractured zones
GEOCHEMISTRY AND TRANSPORT	Simulate chemical species and disequilibrium indeces of natural groundwater		Simulate effects of pressurized dissolved gases on groundwater chemistry near repos.	Simulate effects of complexing on mobilization of radionuclide species; 2 dimensional regional radionuclide transport simulation

Figure 4-2. Program objectives at various repository time stages.

4.3 Geotechnical evaluation

Since a full understanding of the role of groundwater around the repository will be necessary, available experience within the study team will be consulted to provide relevant data concerning, for example, conductivities, flow velocities and temperatures to depths in excess of 500 meters. With regard to the long term nature of the repository and the special considerations necessary due to the heat generation in the spent fuel canisters, special problems will be identified which might be encountered.

The in-situ state of stress of a rock mass is clearly important to the rock mechanics analysis as well as to the hydrogeological conditions which will be analysed. Measurements of stress conditions will be analysed, and use for further deep drill holes, packer tests, and stress measurements will be recommended.

4.4. Thermal loading

The objective of the thermal loading analysis is to calculate the transient temperature distribution in the granitic rock mass as a consequence of the emplacement and containment of heat generating radioactive waste. The analysis will be performed by the finite element method on a two-dimensional model that encompasses the global region of the repository. The input data to the model study will involve the approximate facility geometry, ventilation conditions, and initial thermal loading due to waste emplacement (with thermal power decay); the initial temperature field in the rock mass, the terrestrial heat flow, and the average temperature and convection coefficient at the surface; and the thermal/physical properties of the rock mass, including the thermal conductivity as a function of temperature, the density, and the thermal diffusivity or specific heat. The results will be presented in the form of temperatures as a function of time and position in the model. The transient temperature fields will be used as input to stress and fluid flow model analyses, and to models for evaluation of water chemistry and radionuclide mobility.

4.5. Rock mechanics

The objective of the rock mechanics analysis is to quantitatively evaluate the development of global fracture zones and joint system failure in the granitic rock mass as a consequence of the emplacement and containment of heat generating radioactive waste. The analysis, performed by finite-element methods, will focus on a two-dimensional model that encompasses the global region of the repository, and will be time-dependent in the sense of the thermal behaviour. The development of global fracture zones and joint system failures will be "quasi-static" in the sense of the constitutive laws of rock fracture and joint failure. The degree of fracturing and the associated flow conductivity within the predicted zones must be estimated from the results of laboratory tests on rock core and field observations. The input data to the model study will involve the approximate joint system, facility geometry, and backfilling sequence; the time-and spatially-dependent temperature fields from the thermal loading analysis; the modulus of elasticity, Poisson´s ratio, and coefficient of thermal expansion of rock mass and backfill material; the Mohr envelope of failure for intact rock, residual strength of fractured rock, and shear and deformational characteristics of the joint planes; and the estimated states of in-situ stress and initial pore pressure.

The results will be presented in the form of stresses, displacement, and contours of potential fractured zones as functions of time and position in the model. The transient states of stress and zones of failure will form input to the fluid flow model analysis. Since the rock failure will be a function of the effective stress, the stress and fluid flow analyses may require cycling over specified time intervals in order to effect approximate coupling.

4.6. Groundwater flow field

The objective of the groundwater flow field analysis is to develop a regional flow model of the hydrological regime, which may be affected by the repository and possibly be subject to contamination in the long term.

The data required includes estimates of the hydrogeological properties of the subsurface regions. Field and drillhole data on groundwater pressures and velocity fields will be used where available, including fresh/salt water interface or transition locations. The detailed description and sequence of the repository construction will be required. The geological studies should provide possible scenarios for long term perturbations due to major environmental or geological changes. The effects of these on the groundwater field can be assessed.

The approach during the virgin or preconstruction period would be to use two-dimensional steady state equivalent porous continuum models. The models will include a fresh/salt water interface and be capable of including discrete features if necessary. This model would then form the basis for subsequent near field and long term models.

In order to follow the flow field through the construction period, it will then be necessary to use a transient model of the near field region. This could be a sub-structure of the regional model, and also it will be appropriate to use an equivalent porous continuum with modified permeabilities and porosities in the repository room area to amount for possible fractures and grouting.

The near field transient model could then be extended to the short-term containment period by modifying the room properties to include backfilling and sealing. This model can then estimate the flow fields and duration of the inflow and recharge periods which will probably provide containment in that time. The thermal and rock mechanics simulation results will then be used to modify the flow periods during the heat generating period which will overlap the recharge period. The temperature fields will be used to include thermal convection effects on the flow field and the rock mechanics will allow prediction of potential rock fracture zones which may modify the hydraulic properties.

The long term flow field will be assessed using the two-dimensional steady state regional model used previously for the virgin state, together with the substructure model for non-steady state near field studies. These models could be extended to estimate travel times for non-retarded isotopes.

4.7. Geochemistry and transport simulations

4.7.1. Simulation of radionuclide mobilization by complexing

The purpose of chemical speciation modelling will be to determine the occurrence of dissolved species in natural and radionuclide-contaminated groundwater. As model input, estimates of the water salinity and possible radionuclide leach concentrations will be used in conjunction with existing thermodynamic data and stability constants derived from published experimental data. The model will be developed by adaptation of an existing model that is commonly used in studies of inorganic constituents in natural waters. Based on this modelling, it should be possible to evaluate the potential for ligand complexing to cause mobilization of significant concentrations of radionuclide species that would otherwise be viewed as being strongly retarded in the groundwater flow system in the rock mass.

4.7.2. Simulation of effects of pressurized gases on groundwater chemistry

These simulation studies will provide estimates of the changes in groundwater chemistry that will occur as a result of the effects of elevated partial pressures of gases such as dissolved oxygen and carbon dioxide. A geochemical model based on mass-balance, charge-balance, and equilibrium thermodynamic relations will be used to compute water compositions based on estimated mineralogical conditions in the rock mass. Because of the availability of thermodynamic data, the simulations will be limited to non-elevated thermal conditions. Information on the effects of dissolved gases from the repository on the hydrochemical condition will be a necessary input to considerations of radionuclide transport in the fractured rock mass.

4.7.3. Two-dimensional simulation of radionuclide transport in the regional flow field

Based on the results of the two-dimensional groundwater flow modelling described in section 4.6, various cases of radionuclide transport through the flow field will be simulated for non-reactive radionuclides and for the mobilized fractions of reactive species. Integrating this study with the flow modelling will provide for efficient use of numerical grids and parameter inputs. The velocity field obtained from the flow modelling will be used as the main basis for the transport models. The models to be used in this study is the finite-element advective-dispersion continuum model that is now used relatively routinely at the University of Waterloo. It includes the effect of radioactive decay. Distribution coefficients can be specified if desired. This simulation work will enable immediate benefit to be derived from the results of flow field analysis. The model will produce a variety of radionuclide transport patterns for specified flow fields and assigned values of diffusion coefficients, dispersivity, and retardation coefficients. It will enable the importance of the various processes to be identified.

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AB Atomenergi 77-04-05

02. PM angående värmeledningstal hos Jordmaterial
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03. Deponering av högaktivt avfall i borrhål med buffertsubstans
A Jocobsson och R Pusch
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04. Deponering av högaktivt avfall i tunnlar med buffertsubstans
A Jacobsson, R Pusch
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Ulf Lindblom
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07. Resteffekt för KBS del 1
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08. Utlakning av franskt, engelskt och kanadensiskt glas med högaktivt avfall
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09. Diffusion of soluble materials in a fluid filling a porous medium
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