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Evaluation of the Thermal Effect in a KBS-3 Type Repository

A Literary Survey

Patrick Goblet
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A Literary Survey

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Preface

The Swedish Nuclear Fuel and Waste Management Co., SKB, presented in its latest RD&D Programme, 1998, the ongoing scientific work related to thermal effects in a KBS-3 repository. The programme shall in accordance with the Act on Nuclear Activities be reviewed by the Swedish Nuclear Power Inspectorate, SKI.

In preparation for upcoming reviews of RD&D Programmes and licence applications SKI has decided to compile an updated overview of existing thermal studies related to the KBS-3 and similar concepts. Professor Ghislain de Marsily, member of the French Academy of Science and Dr. Patrick Goblet, Ecole des Mines de Paris have performed this literary survey.

The report provides an overview of the existing thermal studies in high-level nuclear waste disposal, based on the available literature assembled during the survey. Although the emphasis is on a granitic repository, some results obtained by experiments or numerical analyses of other rock types (essentially clay or volcanic tuffs) are also given.

A general conclusion from this work is that thermal calculations constitute the straightforward part of the much more general problem of the hydro-thermo-mechanical behaviour of a geological host rock under the influence of a heat-producing repository.

A possible follow up work based on this study is to perform additional thermal calculations using available analytical tools, in order to corroborate the SKB results.

Stockholm, August 30, 2000

Öivind Toverud

Summary

This report provides an overview of the existing thermal studies in high-level nuclear waste disposal, based on the available literature assembled during this survey. Although the emphasis is on a granitic repository, some results obtained by experiments or numerical analyses of other rock types (essentially clay or volcanic tuffs) are also given.

It is well known that high-level nuclear wastes (spent fuel or vitrified reprocessed waste) generate a great amount of heat, whose power decays with time as the radionuclides decay. Because of this heat output, it is generally accepted that waste cannot be placed in a repository immediately after extraction from a reactor but must be stored for some tens of years in a temporary storage unit before disposal. Even after this temporary storage, the residual heat production is expected to produce a raise of temperature in the near as well as the far field. This temperature raise must be evaluated, because it impacts on other aspects of the repository evolution.

Excessive heat loading can generate mechanical failure of the rock, chemical degradation and transformation of the buffer and rock, water vaporisation and condensation. In many countries, a maximum temperature of less than 100°C has been selected, in order to avoid these difficulties. If the repository is backfilled and resaturated, the heat load can generate convective movement of the water and therefore, transport of dissolved elements away from the repository. Given that the heat generated by the wastes decays with time, the maximum temperature at the repository level is generally reached after a few hundred years, but even if the temperature starts to decrease, the total heat loading of the rock formation continues to increase, until the temperature front reaches the upper boundary of the system (the rock surface) and releases the heat into the atmosphere. The total heat load of the host rock typically starts to decrease only after about 10,000 years. The mechanical effects can therefore peak long after the maximum temperature has been reached. The surface deformation of the rock by expansion (on the order of 1 m above a repository) is often reached at such large times.

Another thermal problem examined in some repository studies is the effect of climate variations at the surface. A glaciation scenario, for instance, would decrease the temperature at the surface, perhaps generate permafrost deep in the ground, that could potentially interact with the thermal pulse from the repository.

The maximum heat loading in a repository is an important design parameter when the extent of a repository is determined, given the amount of waste and the age at which this waste must be disposed. To determine this heat loading, it is necessary to define either the maximum acceptable temperature at the buffer-rock contact, and/or at the outer boundary of the canister. Design options include the nature and dimension of the buffer zone, its water saturation (in the case of clay) and the distance between canisters.

The temperature distribution in the host rock, in the buffer and inside the waste package can be determined by thermal calculations, if the density of waste in the repository is known, as well as the geometry of the disposal option, the properties of the buffer and the host rock and potential gaps between the canister and the rock. These calculations can be made with different degrees of sophistication, e.g. in 1, 2 or 3 dimensions, and with constant or variable material properties (variable water saturation of the medium, thermal properties varying with temperature, etc). The heat transfer is generally assumed to occur mostly by conduction, but in some cases, vaporisation and condensation of water with a large "heat pipe" effect must also be considered. In simple cases, analytical solutions can be used, but generally, numerical techniques are preferred, in particular when other processes are coupled with the temperature in the model : mechanical effects, geochemical effects, hydrological effects.

In this review, the source of information is mostly "grey literature", i.e. technical reports. In order to thoroughly cover such reports, the following organisations and countries were contacted :

-SKB, SKI, Sweden;
-POSIVA, Finland;
-CEA, ANDRA, France;
-DOE and NRC, US
-AECL and Ontario Hydro, Canada;
-NAGRA, Switzerland;
-ENRESA, Spain
-CEN-SCK and ONDRAF, Belgium
-QUANTISCI, England (and Japan)
-NEA/OECD
-CEC - DGXII, Brussels.

A general conclusion from this work is that thermal calculations constitute the "easy" part of the much more general problem of the hydro-thermo-mechanical behaviour of a geological host rock under the influence of a heat-producing repository.

We have examined contributions from various countries, whose repository concepts are quite similar in principle, but different in their details: containers may be stacked in boreholes, lined up horizontally in drifts, or buried in a buffer material in rooms. This does not greatly modify the general modelling approach.

It is clear that at their present stage of development, models are not able to simultaneously cover all the scales, from the regional to the near-field: choices must be made as to what scale is appropriate for a particular aspect. Generally, a very detailed model must be restricted to a local region, which is either a sub-domain of a more general model, with boundary conditions extracted from this regional model, or bounded on the basis of symmetry considerations. In any case, the vertical extent of this local model must be sufficient to include realistic boundary conditions. In a regional model, it is possible to use a simplified representation of the source without loss of accuracy. The development of specific models for various scales, although cumbersome, may have advantages, because one is forced to correctly assess the orders of magnitude of various mechanisms to make the appropriate approximations.

The Equivalent Continuous Medium approach is well suited to the modelling of heat transfer, because this phenomenon is rather insensitive to the presence of fractures. Fractures must, however, be taken into account when the effect of heat on water trajectories is assessed. Generally, the density coupling for sparsely-fractured rocks is a one-way coupling: heat transfer is insensitive to the flow in fractures, but the flow in fractures can be modified by the temperature long after the thermal perturbation of the medium has vanished.

Various numerical techniques are available to solve the heat transfer equation: Finite Elements, Finite Differences, Distinct Elements or even analytical techniques. These techniques have different abilities to deal with coupled mechanisms, but perform equally well for the heat diffusion equation. Thus, the results do not seem to depend greatly on the modelling techniques, because the heat conduction equation is rather robust and not prone to unstable solutions.

There seems to be little uncertainty regarding the value of thermal parameters (thermal conductivity and specific heat of the various materials), and as a consequence, little uncertainty regarding the results of thermal calculations in terms of temperature. This is especially true for saturated media. The major source of uncertainty in the predictions seems to be the behaviour of the bentonite, with respect to its water content : the saturation of the bentonite strongly affects its thermal conductivity, and furthermore, if the bentonite is only partly saturated, two-phase transport of water and heat can occur, making the modelling and predictions much more complex. More precisely, the variation in water content is difficult to predict with accuracy, which impacts on the thermal calculations. The possible existence of a scale effect has been proposed to explain discrepancies between field measurements and predictions based on parameters measured in the laboratory. However, this scale effect has, so far, not been demonstrated for thermal parameters, as is the case e.g., for the hydraulic conductivity.

The most elaborate modelling work found during this review seems to have taken place in Sweden: the concepts used in the various modelling exercises examined here are consistent, except for minor differences in parameters, and reflect the increasing power of numerical tools.

A large body of experimental evidence has been and still is being developed around the hydro-thermo-mechanical aspects. These experiments cover a variety of spatial and temporal scales. The modelling results obtained in connection with these experiments are generally in good agreement with the observations as far as temperature is concerned. At present, the most elaborate work (excluding the US programmes which concern a different hydrological situation) seems to be the FEBEX experiment, on the behaviour of the bentonite buffer.

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1. Introduction

This report provides an overview of the existing thermal studies in high-level nuclear waste disposal, based on the available literature assembled during this survey. Although the emphasis is on a granitic repository, some results obtained by experiments or numerical analyses of other rock types (essentially clay or volcanic tuffs) are also given.

It is well known that high-level nuclear wastes (spent fuel or vitrified reprocessed waste) generate a great amount of heat, whose power decays with time as the radionuclides decay. Because of this heat output, it is generally accepted that waste cannot be placed in a repository immediately after extraction from a reactor but must be stored for some tens of years in a temporary storage unit before disposal. In Sweden, this temporary storage is done in CLAB, a wet storage unit of pools built near Oskarshamn, about 30 m below ground.

The initial heat output of the waste is a function of the burn-up, and also of the fuel type. If MOX (Plutonium and Uranium Oxides) fuel is used, for instance, instead of Uranium Oxides, the heat output is much higher, and the rate of decay is much slower (as will be shown below).

The temperature distribution in the host rock, in the buffer and inside the waste package can be determined by thermal calculations, if the density of waste in the repository is known, as well as the geometry of the disposal option, the properties of the buffer and the host rock and potential gaps between the canister and the rock. These calculations can be made with different degrees of sophistication, e.g. in 1, 2 or 3 dimensions, and with constant or variable material properties (variable water saturation of the medium, thermal properties varying with temperature, etc). The heat transfer is generally assumed to occur mostly by conduction, but in some cases, vaporisation and condensation of water with a large “heat pipe” effect must also be considered. In simple cases, analytical solutions can be used, but generally, numerical techniques are preferred, in particular when other processes are coupled with the temperature in the model : mechanical effects, geochemical effects, hydrological effects.

The maximum heat loading in a repository is an important design parameter when the extent of a repository is determined, given the amount of waste and the age at which this waste must be disposed. In a few cases, “excessive” heat loading has been suggested; this requires that the repository be kept open and ventilated for a significant period of time, to extract the heat, until conduction becomes sufficient to distribute the heat in the host rock. To determine this heat loading, it is necessary to define either the maximum acceptable temperature at the buffer-rock contact, and/or at the outer boundary of the canister. Design options include the nature and dimension of the buffer zone, its water saturation (in the case of clay) and the distance between canisters.

Excessive heat loading can generate mechanical failure of the rock, chemical degradation and transformation of the buffer and rock, water vaporisation and condensation. In many countries, a maximum temperature of less than 100°C has been selected, in order to avoid these difficulties. If the repository is backfilled and resaturated, the heat load can generate convective movement of the water and therefore, transport of dissolved elements away from the repository. Given that the heat generated by the wastes decays with time, the maximum temperature at the repository level is generally reached after a few hundred years, but even if the temperature starts to decrease, the total heat loading of the rock formation continues to increase, until the temperature front reaches the upper boundary of the system (the rock surface) and releases the heat into the atmosphere. The total heat load of the host rock typically starts to decrease only after about 10,000 years. The mechanical effects can therefore peak long after the maximum temperature has been reached. The surface deformation of the rock by expansion (on the order of 1 m above a repository) is often reached at such large times.

One additional mechanism, which is linked to the thermal regime of the repository, is the coupled effect of the thermal gradient on the transport of water (thermal osmosis) and solute (thermal diffusion). Some work has been done to quantify these “non diagonal effects” in the literature, based on the theory of irreversible thermodynamic processes.

Another thermal problem examined in some repository studies is the effect of climate variations at the surface. A glaciation scenario, for instance, would decrease the temperature at the surface, perhaps generate permafrost deep in the ground, that could potentially interact with the thermal pulse from the repository.

In this review, the source of information is mostly “grey literature”, i.e. technical reports. In order to thoroughly cover such reports, the following organisations and countries were contacted :

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-CEN-SCK and ONDRAF, Belgium
-QUANTISCI, England (and Japan)
-NEA/OECD
-CEC - DGXII, Brussels.

The list of examined reports is provided at the end.

2. Aspects to be addressed

In earlier Swedish Performance Assessments (KBS-3, SKB 91, Project 90), all temperature modelling work was based on the thermal analysis of a KBS-3-type repository carried out by Tarandi (1983) [121] and the data presented in his report. In April 1997 the Swedish Nuclear Power Inspectorate completed the SITE-94 performance assessment project. The overall rationale for carrying out SITE-94 was that it should assist SKI in preparing for the licensing of a repository for spent nuclear fuel by building up the necessary review capacity and supporting knowledge.

In SITE-94, different repository-induced temperatures were analysed in order to study the far-field rock-mechanical responses to repository heating followed by the mechanical loading by an ice sheet in the Central Scenario. In the near field, estimates of the decay of heat and temperatures were taken into account when considering both the geomechanical evolution of the rock and the geochemical evolution of the system. The repository temperatures, estimated in each of these studies, vary somewhat according to the type of model, the assumptions and the intended end-use of the calculated temperature values. In these studies, the heat generated by the wastes is modelled with a source term that decays with time.

Future temperature modelling work should strive to use a consistent approach when considering geomechanical and geochemical impacts in both the near and the far field: mechanisms considered, parameter values, numerical techniques, etc.

The objective of this report is to compile and evaluate the current (national and international) knowledge of heat propagation and its impact on repository performance. In this section, we discuss the various viewpoints from which we have analysed the available literature.

2.1. Modelling

Modelling of the thermal behaviour of a repository and its different components is the focus of this study. Modelling approaches are used in various contexts:

- Generic studies, providing a general analysis of the important mechanisms and giving orders of magnitude of thermal effects. Several international cooperation programmes have served this purpose in recent years (PAGIS programme (ref. [23]), DECOVALEX I (ref. [83]) and II (ref. [84]), etc.).
- Modelling in relation to an experimental programme : these studies generally have a more restricted focus, but allow models to be directly compared with reality.
- Site-specific modelling : this type of study tries to represent as accurately as possible the conditions of a real repository.

2.2. Modelling approaches

Fractured media are modelled according to three main approaches:

- Equivalent continuous medium: the porosity and hydraulic conductivity structure related to fractures is not described in detail, but approached through parameters averaged on an Elementary Representative Volume.
- Discrete fracture networks: the fractures are explicitly represented, generally by simple geometric shapes (planar discs or rectangles), sometimes in more detail, through a discretized formulation. It is generally implicit that fractures play the dominant role in water circulation; hence, the permeability of non fractured blocks is considered negligible.
- Distinct Element Approach: the solid blocks are explicitly represented, and the role of fractures is to transmit mechanical constraints between blocks. This approach is specifically oriented towards the description of the mechanical behaviour of a rock mass.

All three approaches have been used in the references that we have consulted. We shall try to determine the implications of the choice of method for the modelling results. The dimensionality of the models is also discussed.

2.3. Numerical technique

The numerical tools are described. Here again, the goal is to examine how the use of a particular model impacts on the results.

2.4. Scale

The spatial scale of available studies ranges from the very local (laboratory experiments on rock or buffer samples) to the regional scale (global site model). Much work is being done on the near field (effect of bentonite saturation, etc).

The temporal scale covers “short-term” (core experiments), “local-time scale” (thermal phase limited to a few thousand years) and “global-time scale” (climate cycles).

2.5. Mechanisms

Studies are available concerning the various components of the confinement system: source term (heat propagation in the container system and resulting thermal output), buffer behaviour (effect of heat on clay properties, moisture distribution) and rock mass behaviour (conductive heat transfer, convection, radiation, mechanical effects).

2.6. Parameter values

Thermal parameters are reviewed, with particular emphasis on the following aspects: origin of values, variability, uncertainty.

Parameter acquisition methods are also discussed; when possible, the various techniques used to measure parameters are compared.

3. Mechanisms of heat propagation

In this section, the main mechanisms of heat propagation in geologic media are briefly reviewed in order to provide a general framework. The presentation is essentially inspired by ref. [15]. This book, which deals with many important issues related to thermal mechanisms in waste disposal, is in French. We will therefore give a short overview of its contents:

- Thermal mechanisms in geotechnics (P.Berest)
- Basics of thermomechanics (P.Berest, G.Vouille)
- Heat propagation in the soil and geothermal flux (G.Vasseur)
- Modelling of thermal and hydraulic fluxes in natural media. Practical considerations (G.de Marsily)
- Modelling of structures under thermal constraints (S.M.Tijani)
- Thermomechanical aspects related to geological disposal of nuclear waste (B.Come, S.Derlich, D.de Bruyn, T.Hueckel, G.Staupendahl, J.P.Charpentier, M.Ghoreychi)
- Finite-Element modelling of structures under thermal constraints. Application to geological disposal of radioactive waste (P.Jamet, A.Millard)
- Rock and soil behaviour at low temperature (D.Blanchard, M.Fremond, M.Levy)
- Calculation techniques used for soil freezing (P.Gonze)
- Recent data on rock behaviour with temperature (R.Houpeurt, F.Homand-Etienne)
- Brittle-fracture mechanics under thermomechanical constraints (P.Jouanna, G.Berthomieu)

3.1. Mechanisms

The description of heat propagation in an immobile medium is based on an experimental law (Fourier’s law) and a conservation equation.
The Fourier law relates the heat flux φ_c across a unit surface to the temperature gradient through the relation:

$$\overrightarrow{\varphi_c} = -\Lambda \overrightarrow{\mathrm{grad}\,\theta} \qquad (1)$$

φ_c is the conductive flux (W/m^2), θ the temperature (^{o}C), and Λ the thermal conductivity of the medium (W/m^{o}C).
The heat conservation law is:

$$\mathrm{div}\varphi_c + \rho C \frac{\partial \theta}{\partial t} = 0 \qquad (2)$$

ρ is the medium density (kg/m^3), and C the specific heat capacity (J/kg^{o}C). *t* is time.

In a composite medium, such as a porous medium containing water, one must use average thermal properties that combine the properties of each component. The rules for this combination are not always straightforward. Generally, a volumetric weighting (through porosity) is used:

$$\Lambda_t = \omega\Lambda_w + (1-\omega)\Lambda_r \qquad (3)$$

Λ_t is the total conductivity, Λ_w and Λ_r the conductivities of water and solid rock. ω is the total porosity. Likewise:

$$(\rho C)_t = \omega(\rho C)_w + (1-\omega)(\rho C)_r \qquad (4)$$

When the interstitial water is mobile, a second heat transfer mechanism sets in: heat is advected with the water. This leads to a modified equation:

$$\mathrm{div}(\varphi_c + \varphi_a) + \rho C \frac{\partial \theta}{\partial t} = 0 \qquad (5)$$

φ_a is the advective flux (W/m^2), expressed as

$$\varphi_a = (\rho C)_e U_D \theta \qquad (6)$$

U_D is the Darcy velocity.
Finally, a third mechanism of heat propagation is the dispersive flux. Dispersion is due to the fluctuations of the local Darcy velocity around the average value defined by U_D. The dispersive flux is classically expressed by a Fourier-type law:

$$\varphi_d = -\Lambda_d \mathrm{grad}\theta \qquad (7)$$

Where Λ_d is an apparent conductivity, expressed in tensor form as a function of the Darcy velocity:

$$\Lambda_d = \bar{\bar{\alpha}}\,|U_D| \qquad (8)$$

$\bar{\bar{\alpha}}$ is the dispersivity tensor (m), which may have different components in the direction of velocity and in the transverse directions. It is generally admitted that, for the low velocities considered in the present work, the dispersive flux is negligible compared to the conductive flux.
Introducing the dispersive flux into the conservation equation leads to:

$$\mathrm{div}(\varphi_c + \varphi_a + \varphi_d) + \rho C \frac{\partial \theta}{\partial t} = 0 \qquad (9)$$

Or, replacing each flux by its expression:

$$\mathrm{div}\left\{\left(\Lambda_t + (\rho C)_w \bar{\bar{\alpha}} U_D\right)\mathrm{grad}\theta - (\rho C)_w U_D \theta\right\} = \rho C \frac{\partial \theta}{\partial t} \qquad (10)$$

3.2. Boundary conditions

Equation (10) may be solved provided that the initial and boundary conditions are appropriate. The initial state is defined by a temperature distribution in the region of interest. Boundary conditions are generally expressed as:

- Prescribed temperature: this occurs when a domain is in contact with a continuously flowing or mixing fluid, such as the atmosphere or a large fluid body
- Prescribed heat flux: this condition describes, for instance, the geothermal flux or the heat flux generated by the waste containers
- Radiation: this condition describes a heat transmission through a thin fluid boundary layer.

Note that the appropriate boundary condition for a given problem may depend on the scale of analysis: for example, the heat-flux condition is sufficient to describe the influence of the thermal load on the surrounding rock, but a detailed description of the temperature distribution near the canister may require a simultaneous solution of the heat transfer equation in the canister and the surrounding media. Likewise, the detailed description of the heat load history may be useless for predictions on the scale of several thousand years, because at this scale the source term appears instantaneous.

3.3. Parameters

A range of variation for the thermal parameters (conductivity and specific capacity) is proposed in ref. [15]. For granite, the range is 1.2 to 4 W/m^{o}C for the conductivity, 0.5 to 1 kJ/kg^{o}C for the specific heat. This is a very narrow range compared to those of other parameters such as hydraulic conductivity.

The conductivity of a composite material may be computed with simple formulae when the materials are combined according to a simple geometry: for instance, for two layers of different materials piled up in the direction of the thermal gradient, the equivalent conductivity is the harmonic mean of the individual conductivities. If the thermal gradient is parallel to the layers, the equivalent conductivity is the arithmetic mean. This type of averaging approach is proposed e.g., in [6] and [126].

This might lead to an important variation of granite conductivity when open, dry fractures are present, because air has a much lower conductivity. This is rare in natural conditions, because the mechanical stress prevents the fractures from opening.

The thermal parameters show little variation either with temperature or with pressure. The main sources of variations are the water content (for argillaceous materials) and the appearance of open fractures.

3.4. Couplings

Thermal transfer may, to some extent, depend on hydraulic and mechanical mechanisms: the water flow is modified by temperature because of density and viscosity variations of the water. This, in turn, may modify the advective temperature flux. Similarly, mechanical effects caused by the temperature may modify the thermal parameters. This thermo-hydro-mechanical coupling is a complex problem. However, it becomes very much simpler when one is only concerned with temperature, because:

- The advective heat flux is generally negligible compared to the conductive flux.
- The variation of thermal parameters is negligible.

For these reasons, temperature propagation appears as a quasi-independent mechanism, which can be modelled separately.

Let us finally mention "non diagonal" couplings, discussed by Marsily in [15]: heat flow due to a hydraulic gradient (thermal filtration), an electric-potential gradient (electrophoresis) or a concentration gradient (Dufour effect). These effects are, at present, thought to contribute negligibly to the heat transfer. Inverse effects, such as the Soret effect, coupled with buoyancy effects, might contribute significantly to the solute transfer. This is discussed in, for example, [77] and [44].

In a recent study (ref. [123]), the coupled effects of the thermal loading of a clay-marl repository was analysed by a simplified modelling of the coupled heat, fluid flow, and solute transport. The author assumes that the peak of the thermal output is passed at, for instance, 1,000 years. He reviews the available coupling coefficients in the literature, and concludes that very few measured parameters are available, and that only scoping calculations can be made at this stage. He suggests that the major coupled mechanism is thermal osmosis (water movement in the thermal field towards the heat source). He also considers thermal diffusion, hyperfiltration and chemical osmosis. His modelling results indicate that the thermal osmosis effect is, however, counter-balanced by the geometry of the system : when water flows towards the heat source because of the thermal gradient, the hydraulic pressure increases at the heat source, and the hydraulic gradient counter-acts the thermal gradient, resulting in a zero increase of velocity. He concludes that coupled processes, at least after the thermal peak, are not very important in a performance assessment. However, this calculation was done under the assumption of a homogeneous medium, and it is also shown that if e.g., a fracture makes the medium heterogeneous, the two gradients may not, in some cases, work against each other (water could flow towards the heat source in the unfractured medium and away form the heat source by the hydraulic gradient in the fracture, with a non-negligible net effect). Similar conclusions were reached at Yucca Mountain ([7], [63])

It must be pointed out, however, that most of these studies on coupled properties rely on the Onsager principle of irreversible thermodynamics, which specifically assumes that there is no electrical fields in the medium. Since there are always in natural media, and even more so if pieces of metal are introduced into the medium (e.g. a metal canister), spontaneous electrical potentials which can easily be measured, the theory is not directly applicable and cannot be used straightforwardly. Additional theoretical work may be required here.

3.5. Conclusion

Let us end this short review of thermal mechanisms in geologic media by two quotations from ref. [15]:

> *In almost all cases, thermal calculations give results in very good agreement with observations. This is sufficiently rare in geotechnics to deserve being underlined (P.Berest)*
>
> *Finally, one must note that there is generally excellent agreement between calculations and measurements concerning heat propagation in geologic media (B.Come)*

These observations, which are confirmed by our review, are a key result of this work: the modelling of possible temperature evolution around a repository seems to be much more robust and reliable than other aspects (e.g., prediction of water velocity, mechanical behaviour of a rock mass, general THM coupling).

4. Comparison of various modelling approaches

4.1. Sweden

It may be useful to try to put in historical order the various referenced documents concerning the Swedish approach to thermal problems.

Tarandi (1983, SKB TR 83-22)

Tarandi's work ([127]) is the basic reference for thermal modelling related to a repository. The modelled geometry is as follows :

- depth of the repository : 500 m
- repository composed of tunnels with variable spacing (25-60 m), inside which boreholes with an average spacing of 6 m (variation 4.3 to 8 m) contain the 4.7 m high canisters. A one-layer and a two-layer design, the latter with a spacing of 100 to 250 m between planes, are considered.

Thermal loading obeys a piecewise-exponential variation with time. The initial loading per canister is 850 W.

The heat transfer mechanism is pure conduction. A zero initial temperature is assumed everywhere, which implies that a temperature increase, and not an absolute temperature, is computed. Due to the relatively limited computing resources available at the time of the study, a simplified approach was devised : a global one-dimensional model (from ground level down to a depth of 4000 m) is used to describe the temperature profile along a vertical axis through the repository centre. A finer local model describes a two-dimensional, vertical cross-section through a gallery (scale 15 x 20 m). Boundary conditions for this model are extracted from the global model. Finally, a steady-state analytical temperature distribution is computed for a single canister. A three-dimensional model is proposed as well. The numerical codes are based on Finite Differences.

The thermal conductivity of the host rock is constant and at 3 W/m/^{o}C, with two variants : 2 W/m/^{o}C and 3.6 W/m/^{o}C. The thermal conductivity of bentonite is assumed to vary with water content in a simple manner : 0.75 W/m/^{o}C for the first 150 years (dry conditions), and 1.5 W/m/^{o}C afterwards (saturated conditions). The specific heat of the rock varies between 1.8 and 2.5 MJ/m^3/ ^{o}C (average value 2 MJ/m^3/^{o}C), and is 2.2 MJ/m^3 ^{o}C for bentonite.

Thunvik & Braester (1991, SKB TR 91-61)

This work ([128]) deals basically with the same topic as Tarandi's (1983), but with some differences regarding parameters and modelling approaches. The basic geometry is the same : KBS-3-type repository, depth of 500 m, single-layer design, tunnel spacing 20 - 30 m, borehole spacing 3 – 6.2 m. The initial heat load per canister is 1066 W instead of 850 W, in accordance with the SKB-91 specifications. Its subsequent evolution follows the same type of piecewise-exponential law.

Taking advantage of increased computational capacity, the geometrical description is fully 3-dimensional. The modelled zone extends from the surface down to 1000 m below the repository and, owing to symmetry considerations, it is restricted horizontally to an elementary zone in the vicinity of a single canister, bounded by three vertical symmetry planes: two that cross the longitudinal symmetry axis of the canister, the third one midway between two boreholes.

The near-field description includes the canister, represented as a homogeneous volume with average material properties, the bentonite buffer around the canister, the backfilling and the host rock.

The heat transfer mechanism is conduction. An initial temperature field is imposed, according to a vertical gradient of 13 ^{o}C/km, with a surface temperature of 5.8 ^{o}C. The thermal conductivity is 3 W/m/^{o}C for rock, 2.4 W/m/^{o}C for backfill and 0.75

W/m/^{o}C for bentonite (corresponding to dry conditions). The specific heat of the rock is 2.2 MJ/m^3 ^{o}C, 3 MJ/m^3 ^{o}C for backfill and 2.2 MJ/m^3 ^{o}C for bentonite.

The calculation method is based on a Finite-Element solution of the heat conduction equation.

On the whole, this work is consistent with Tarandi's work, but makes use of a more recent canister specification and of a higher computing capacity. The conclusions of this work form the basis for thermal calculations in Project 90 ([120]).

Hökmark (1996, SKB AR D-96-014)

This work ([67]) is a local-scale analysis of a subregion of the repository including a tunnel length of 54 m and 6 deposition holes. The thermomechanical modelling uses the Distinct Element technique. The thermal part of the analysis is based on a semi-analytical approach, whereby the heat sources are represented by a superposition of point sources. The underlying hypotheses are : homogeneous medium (the influence of the canister and the buffer is neglected), depth 450 m, tunnel spacing 25 m, borehole spacing 6 m. The thermal loading varies with time according to a law which is close, but not similar, to the law used in Tarandi (1983) and Thunvik & Braester (1991). The initial load is 1050 W / canister. The total number of canisters is 5285. The thermal parameters are similar to those used by Thunvik & Braester (1991) : 3 W/m/^{o}C for the conductivity, and 2.1 MJ/m^3 ^{o}C for the specific heat.

Hansson et al. (1995, SKI 95 :40 and SKI 95 :41) and Shen et al. (1996, SKI 96 :17 and SKI 96 :18)

This series of reports ([61],[62],[118],[119]) deals with the more general aspect of the effect of thermal loading on the rock stability. However, part of the work is devoted to the calculation of temperature variations. This work is a part of the SITE-94 project.
The geometry of the repository is classical (depth 500 m, tunnel spacing 25 m, borehole spacing 6 m). The heat-loading variation follows the formula proposed by Thunvik & Braester (1991) for the first 1,000 years and subsequently, follows a new exponential expression. The initial load is 1,066 W per canister. The total number of canisters is 400 (SITE-94 concept) and 4,000.

The properties of the canister and buffer are not taken into account. The thermal material properties of the rock are 3 W/m/^{o}C (conductivity) and 2 MJ/m^3 ^{o}C (specific heat).
The initial temperature profile is described by a surface temperature of 6 ^{o}C and a vertical gradient of 16 ^{o}C/km, resulting in 14 ^{o}C at repository level.

The mechanical calculations use the Distinct-Element technique. However, the thermal calculations are based on a semi-analytical approach : point sources are superimposed to describe the spatial extent of the source and its temporal variation.

While computed or measured temperature profiles are generally very smooth, the temperature profiles shown in this study have a jagged shape, whose origin is not clear to us, since the material is supposed to be homogeneous.

Claesson and Probert (1996, SKB TR 96-12) and Probert and Claesson (1997, SKB TR 97-27)

These two authors ([29],[103]) suggest that the temperature field be calculated with an analytical formulation rather than a numerical technique. The analytical formulation is developed in the first reference. It is based on pure thermal conduction. To allow an analytical solution, the medium has to be considered homogeneous. No distinction is therefore made between the thermal properties of the canister, the backfill and the host rock.

In the second report, the approach is applied to a KBS-3 concept. The geometry is consistent with previous work : depth 500 m, distance between tunnels 25 m, distance between boreholes 6 m. The initial thermal load for a single canister is 1,000 W. The subsequent variation with time is consistent with Thunvik and Braester (1991) for the first 1,000 years. A slightly different formulation is proposed after 1,000 years, also formally different from Hansson et al. (1995), but consistent in shape. Finally, the thermal conductivity of the rock is 3 W/m/^{o}C, and the specific heat is 2.2 MJ/m^{3} ^{o}C, in accordance with the value used by Thunvik and Braester (1991).

Israelsson et al. (1997, SKB PR D-97-10)

Thermal calculations are only a part of this report ([75]), devoted to a more general thermo-mechanical approach (discussed also in [60]). The calculations take into account thermal conduction in a homogeneous medium (no distinction between host rock and man-made material). Several geometrical arrangements are considered : one, two or three layers of tunnels, with various vertical distances between layers. In the basic one-layer set-up , the distance between tunnels is in the high range (40 m), while the distance between boreholes is 6 m . Thermal parameters for the host rock are within the usual range : 3 W/m/^{o}C for conduction and 2 MJ/m^{3} ^{o}C for specific heat.

The initial thermal load per canister is significantly higher than in previous studies (2400 W). The reason for this choice is not clear, but could result from an assumption of early disposal.

The thermal conduction equation is solved by a numerical technique.

Ageskog and Jansson (1998, SKB HRL-98-20)

This study ([1]) differs in focus from the previous ones, since it deals with the a priori modelling of an experimental program. It has, therefore, a more limited spatial and temporal scale (5 to 10 years). The geometry is much more detailed than in the studies described above : canister, buffer, backfill and rock are described in detail. The effect of 1 cm gaps between e.g., canister and buffer or buffer and rock can be modelled, which requires an extremely fine Finite-Element discretization.

The basic mechanisms are similar to those of the previous studies. The thermal conductivity of the rock is lower (2.43 W/m/^{o}C) and varies with temperature (2.22 W/m/^{o}C at 100 ^{o}C). The thermal conductivity of bentonite also varies with temperature.
The thermal load varies with time according to the law used in Thunvik and Braester (1991), but with a higher initial value (1800 W / canister).

Parameter	Value	reference
Thermal conductivity of granite	3 W/m/^{o}C (2 – 3.6)	[127]
Thermal conductivity of bentonite	0.75 W/m/^{o}C	[127] (dry conditions)
Thermal conductivity of bentonite	1.5 W/m/^{o}C	[127] (saturated conditions)
Thermal conductivity of granite	3 W/m/^{o}C	[128]REFMERGEFORMAT
Thermal conductivity of backfill	2.4 W/m/^{o}C	[128]REFMERGEFORMAT
Thermal conductivity of bentonite	0.75 W/m/^{o}C	[128] (dry conditions)REF
Thermal conductivity of granite	3 W/m/^{o}C	[67]
Thermal conductivity of granite	3 W/m/^{o}C	[61],[62],[118],[119]
Thermal conductivity of granite	3 W/m/^{o}C	[29],[102]
Thermal conductivity of granite	3 W/m/^{o}C	[75]
Thermal conductivity of granite	2.43 W/m/^{o}C (2.22 at 100 ^{o}C)	[1]
Specific heat of granite	2,2 MJ/m^3/^{o}C	[128]
Specific heat of backfill	3 MJ/m^3/^{o}C	[128]
Specific heat of bentonite	2,2 MJ/m^3/^{o}C	[128]
Specific heat of granite	2,1 MJ/m^3/^{o}C	[67]
Specific heat of granite	2 MJ/m^3/^{o}C	[61],[62],[118],[119]
Specific heat of granite	2,2 MJ/m^3/^{o}C	[29],[102]
Specific heat of granite	2 MJ/m^3/^{o}C	[75]

Table 1: Parameter values used in the Swedish studies (values in parentheses indicate ranges of variation)

4.2. Switzerland

4.2.1. Analysis of Hopkirk and Wagner (ref. [68])

The work presented in this report is a part of the Projekt Gewähr. The calculations are made for a variety of heat-producing waste: High-Level Waste (reprocessing waste and spent fuel) and Intermediate-Level waste (hulls and end-caps, co-precipitation sludges from reprocessing, decommissioning waste).
Two types of repositories are considered: the Type-C repository is designed for HLW and some ILW. The type-B repository is designed for ILW and LLW.

Type-C repository: this repository is sited in granite, at a depth of about 1,200 m. It comprises horizontal galleries, 40 m apart**,** in which the containers are disposed horizontally along the axis and separated by a gap of 7 to 10 m (see fig. *1*). The modelling of this geometry is done at two scales: on the global scale, the effect of axial gaps between the containers is neglected, and a two-dimensional model, perpendicular to the gallery axis and bounded by symmetry planes, is used (fig. *2*). The transient temperature field obtained from this model is used as boundary conditions for a more precise local model, based on a two-dimensional radial approximation around the gallery axis. The components considered in the modelling are: the canister, represented as a medium of uniform thermal properties, the buffer and the rock. The effect of gaps between these components is studied. The heat exchange through these gaps is by conduction and radiation. One gallery at a time is modelled: no influence of other galleries is considered (which is reasonable considering the spacing between the galleries).

The initial temperature of the system is not uniform: a different temperature is used for the rock, the bentonite and the canister. The latter is obtained by a calculation describing the cooling of the canister in a gallery.

The thermal conductivity of granite is taken to be 2.5 W/m/^{o}C, considered as a conservative value as compared to higher values obtained on samples. The thermal conductivity of bentonite is assumed to vary with water content as well as with temperature. However, due to the lack of information on resaturation, only the variation with temperature was actually taken into account, which leads to a conservatively low value of the conductivity.

In the type-C repository, the possibility of storing ILW in concrete silos is also considered. The dimensions of these silos are 40 m in height and 10 m in diameter. They are filled with waste drums and backfilled with cement. When they are full, the gaps between the silos and the rock are filled with bentonite. The modelling of the silos is done by means of a simple one-dimensional radial model.

Type-B repository: in a Type-B repository, ILW and LLW are disposed in horizontal caverns, that are progressively filled up in 50 m sections and backfilled with cement (fig. *3*). This type of repository is supposed to lie at a shallower depth. No particular geologic medium is considered, therefore generic properties are used. The modelling is based on a vertical cross-section through a cavern. Due to the particular loading sequence and the large diameter of the caverns (12 – 14 m), heat is propagated by several mechanisms: conduction, convection by air and radiation. Methods to model the superposition of these mechanisms in a simplified manner are proposed.

4.2.2. Heater test report (ref.[117])

This work reports a heater test performed on the Swiss site of Grimsel: two electrical heaters H1 and H2, each 6 m long, were installed at a depth of 12 m below the floor of an experimental gallery. The distance between the two parallel heaters was about 2 m. These heaters were subjected to a three-year heating programme. The programme included a period of 9 months when H1 operated alone, 9 months of simultaneous operation, a 3-month cooling phase and finally, a 3-month simultaneous heating phase. Each heater reached a temperature of 90 ^{o}C. 127 thermometers measured the temperature field.

At a preliminary stage, the experiment was modelled for dimensioning. A simple axisymmetrical Finite-Element model was used. The thermal conductivity was 3.6 W/m^{o}C. The maximum discrepancy between model and experiment was 6°C. This is considered satisfactory since the actual geometry of the heaters is not precisely modelled. Furthermore, the measurements show evidence of convective flow through a fracture and density effects, mechanisms that are not taken into account by the model.

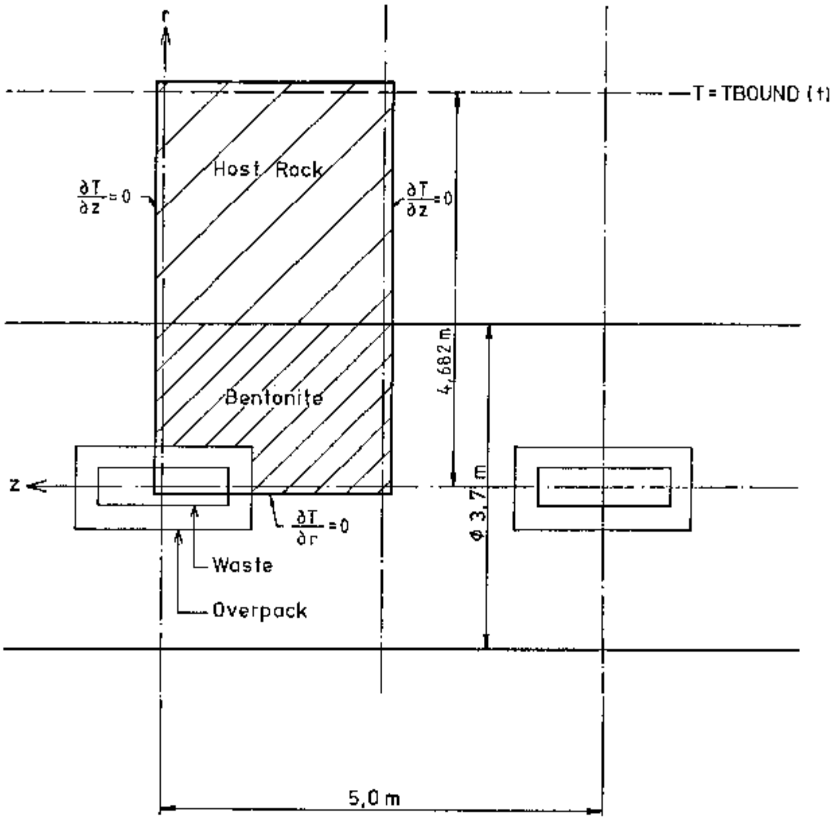


Figure 1: Diametral plane through the axis of a storage tunnel showing (hatched) the domain of the fine scale (cylindrical) model (from [68])

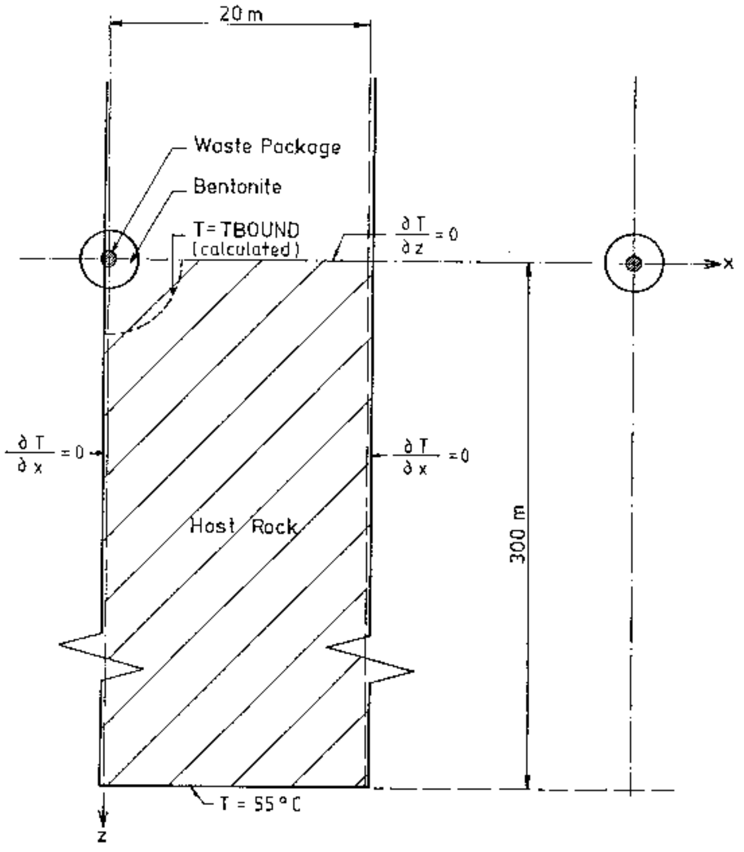


Figure 2: Plane perpendicular to storage tunnel axes showing (hatched) the domain of the coarse scale (Cartesian) model (from [68])

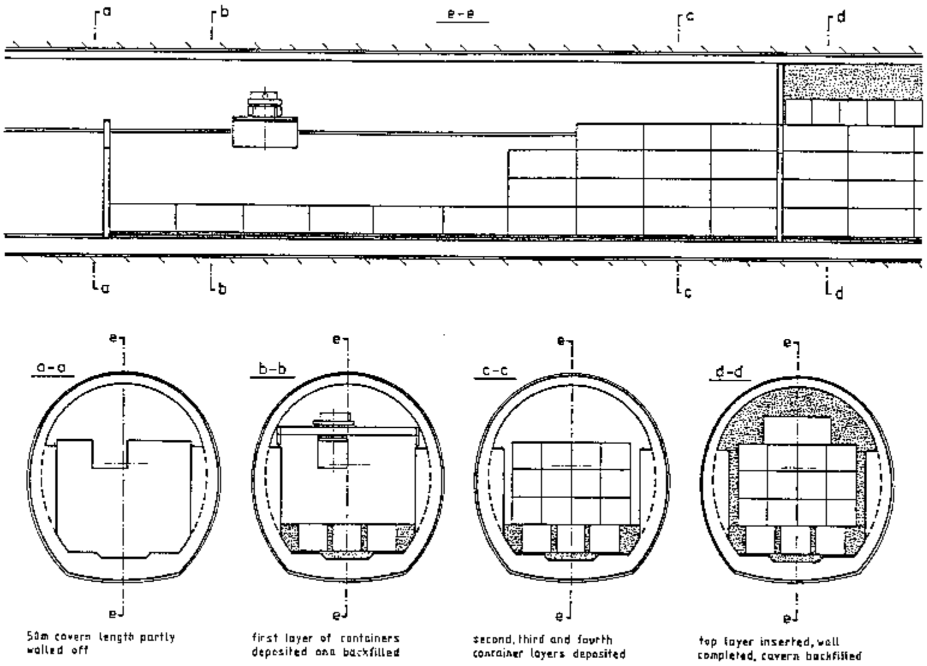


Figure 3: Sectional views of a typical 50 m length of storage cavern in the repository for low and intermediate level waste showing different phases of filling (from [68])

4.2.3. Kristallin-I report (ref. [95])

This report presents a comprehensive description of the post-closure radiological safety assessment of a repository for vitrified high-level radioactive waste, sited in the crystalline basement of Northern Switzerland. Thermal aspects are only briefly discussed in this report:

- The section “Thermal constraints on design” points out the importance of thermal effects. However, the results used here are those of ref. [68], confirmed by more recent calculations.
- The section “The Short-Term Thermal Stability of Bentonite” contains a discussion based on a review of the literature concerning the effect of local desaturation of bentonite, followed by slow resaturation.. The bentonite is not expected to change sufficiently to alter its confining properties.
- Finally, the section “FEPS Related to Long-Term Climatic Changes” discusses the effect of climate cycles. This point is analysed in more detail in section 8.

The limited space devoted to temperature effects in the Kristallin-I report seems to reflect the following point of view: although temperature effects are of primary importance in the assessment of the behaviour of a repository, the present state of modelling, as exemplified in report [68] is sufficient to permit reliable modelling.

4.2.4. Sato et al. (ref. [114])

This report shows dimensioning calculations similar to those by Hopkirk and Wagner ([68]). It is based on a concept close to that of Project Gewähr with the exception of a few characteristics essentially concerning the canister properties and the thermal output.

The repository concept is based on horizontal galleries. The canisters are positioned horizontally along the axes of the galleries and surrounded by compacted bentonite (fig. *4*). The canisters are made of steel with an outer copper shell. The fuel assemblages are packed with quartz sand. Their dimension is 4.8 m (length) × 0.822 m (diameter). The host medium is assumed to be either crystalline (Northern Switzerland basement), or sedimentary (Opalinus clay).

The mechanism taken into account is pure thermal conduction. The corresponding equation is solved with a 3-D Finite Element simulator (ADINA-T). Thermal parameters are considered to be independent of temperature. The effect of water content on the thermal parameters of the bentonite is approximated by globally modifying these parameters. Air gaps between the bentonite and the canister and between bentonite and host rock are simulated. However, radiative thermal flux is not considered, but simulated through an increase of the air conductivity.

The simulated domain is a 3-D elementary volume bounded vertically by symmetry planes (fig. *5*): two vertical planes parallel to the gallery axis (one along the gallery axis, one at mid-distance between two galleries), and two vertical planes perpendicular to the previous direction (one through the canister mid-point, one at mid-distance between two canisters). The vertical extent is 500 m above and below the gallery plane. The inner structure of the canister is represented by a simplified axisymmetric structure: concentric layers represent the fuel, the steel rack, the quartz sand and the steel and copper shells. The thickness of each layer is chosen in such a way as to conserve the volumes.

The base case shows a temperature in the bentonite of between 126^{o}C at the canister contact and 98^{o}C at the host-rock contact. The maximum temperature is reached after about 15 years. A maximum temperature of 100^{o}C is computed after 800 years at the canister/bentonite interface.

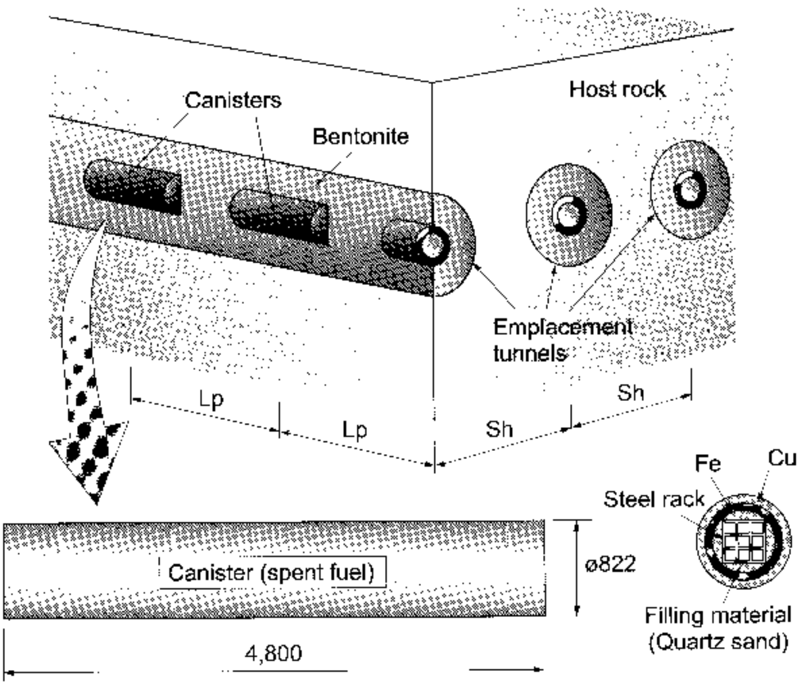


Figure 4: Canisters and emplacement tunnels (dimensions of canister in mm) (from[114])

A number of variations are proposed to test the sensitivity of the results to various parameters:

- Heat generation per canister: the base-case value is 1,000 W. An increase to 1,500 W results in a significant increase in temperatures (plus 22°C at the bentonite/host rock interface).
- Tunnel spacing: the base-case spacing is 20 m. The results are shown to be relatively insensitive to an increase in spacing (temperature decrease of 10°C for a distance of 40 m), but very sensitive to a reduction (temperature increase of 40°C for a 10 m distance).
- Canister pitch: a variation of the longitudinal canister spacing of between 3 m and 7 m causes little difference in the results.
- Thermal properties of the crystalline host rock are varied between 2 and 3 W/m°C (thermal conductivity) and between 1.8 and 2.8 MJ/m°C (thermal capacity). Likewise, the bentonite properties are varied between the following limits: 0.7 W/m°C for the conductivity and 1.1 MJ/m°C for thermal capacity (properties of dry bentonite), 1.7 W/m°C for conductivity and 2.1 MJ/m°C for thermal capacity (properties of wet bentonite). These variations result in limited temperature changes (a few degrees).
- The presence of air gaps causes a small temperature increase.
- Host rock: lower temperatures are calculated for a repository in clay despite the lower thermal properties of clay. This is due to the lower ambient temperature associated with a shallower depth (600 m). For a crystalline host rock (base case depth 1,200 m), a decrease of 10°C is obtained if the depth is reduced to 900 m. This is consistent with the postulated natural gradient (3° for 100 m).

The major conclusion of this study is that the most temperature-sensitive parameters are the gallery spacing and the thermal output.

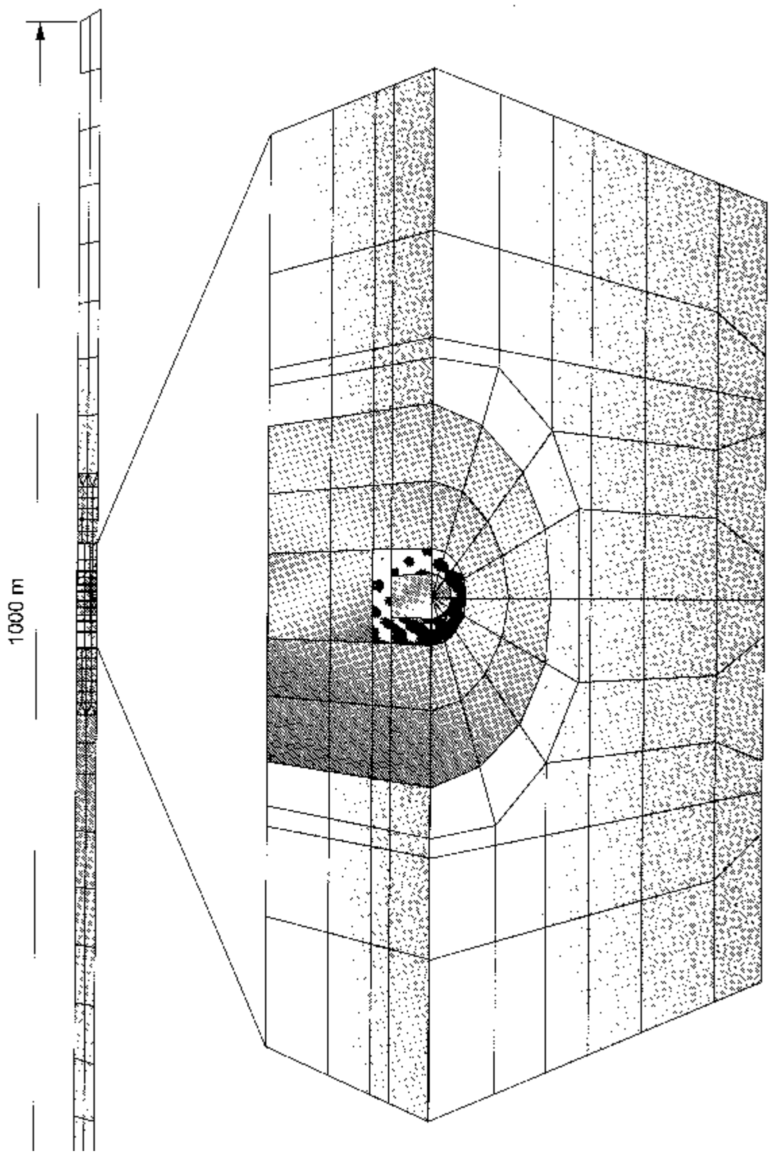


Figure 5: Three-dimensional finite-element mesh (from[114])

Parameter	Value	reference
Thermal conductivity of granite	2.5 W/m/^{o}C	[68]
Thermal conductivity of granite	3.6 W/m/^{o}C	[117]
Thermal conductivity of granite	2-3 W/m/^{o}C	[114]
Thermal conductivity of bentonite	0.7 W/m/^{o}C	[114] (dry conditions)
Thermal conductivity of bentonite	1.7 W/m/^{o}C	[114] (wet conditions)
Specific heat of granite	1.8 – 2.8 MJ/m^3/^{o}C	[114]
Specific heat of bentonite	1.1 MJ/m^3/^{o}C	[114] (dry conditions)
Specific heat of bentonite	2.1 MJ/m^3/^{o}C	[114] (wet conditions)

Table 2: Parameter values used in the Swiss studies (values in parentheses indicate ranges of variation)

4.3. Canada

We begin by discussing two references devoted to generic thermal calculations, and continue with a modelling exercise around the Whiteshell research area.

4.3.1. Generic thermal modelling (Tsui et al., ref. [129],[130])

These two reports present generic 3-D calculations concerning a repository situated in the Canadian shield. Two options for waste emplacement are considered:

- The "borehole" option, where the waste containers are placed in boreholes drilled from the room floor (fig. *6*).
- The "in-room" option, where they are buried in a homogeneous thick layer of buffer material covering the floor of the room (fig. *9*).

The first concept is closest to the Swedish one but the generic approach is common to the two concepts.

The in-room concept uses 8-m wide and 10.5 m high-galleries. A 5 m thick layer of compacted sodium bentonite and silica sand is spread on the gallery floor. The containers are buried in this material. The gallery is then filled to a height of 3.5 m with a mixture of crushed and graded host rock and glacial clay, and the remainder of the room is backfilled with a buffer material (fig. *10*).

The TWPP (Thin-Walled, Particulate-Packed) container is used. Its dimensions are 0.63 m diameter and 2.2 m in height.

Material properties used in the thermal calculations are:

- Thermal conductivity: 3 W/m^{o}C for the rock mass, 1.5 W/m^{o}C for the buffer and backfill, 1.5 W/m^{o}C for the container (modelled as a homogeneous material).
- Specific heat: 845 J/(kg^{o}C) for the rock mass, 750 J/(kg^{o}C) for the buffer and backfill, 500 J/(kg^{o}C) for the container.
- Density: 2,650 kg/m^3 for the rock mass, 1,670 kg/m^3 for the buffer, 2,100 kg/m^3 for the backfill, 3,980 kg/m^3 for the container.

The initial thermal load is 297 W per container, making an average areal load of 11.4 W/m^2 for a pitch distance of 2.6 m between containers and 14.2 W for a 2.1 m distance.

The aim of the calculations is to obtain a detailed 3-D thermal and mechanical response in the near field. To achieve this precision, a “unit-cell” is represented in the calculations. It represents a volume of host rock and gallery, bounded vertically by four symmetry planes: two are parallel to the gallery axis, one at mid-distance between galleries, one along the gallery axis; two are perpendicular to the gallery, one across the containers and one at mid- distance between two container rows. The top boundary is the ground surface, and the bottom boundary is 2,000 m below the gallery level.

The concept of unit cell is valid for containers situated near the centre of the repository, and conservative for containers situated near the repository boundaries.

Boundary conditions are adiabatic on the vertical boundaries and fixed temperatures on the top and bottom boundaries, with an average gradient of 12^{o}C/km.

The Finite-Element code ABAQUS is used for the calculations. A very fine discretization is applied in both studies, particularly in the “borehole” option, which represents the vicinity of the boreholes with great precision: about 10,000 elements and 12,000 nodes are used, the smallest ones approximately 0.15 m × 0.20 m × 0.40 m (fig. *8*, *11*).

Results: for the in-room option, a maximum temperature increase of 83^{o}C is found at the outer container surface after 25 years. This temperature depends strongly on the distance between containers: the temperature increase drops to 70^{o}C when the distance is lengthened from 2.1 m to 2.6 m.

In the borehole option, the sensitivity to borehole distance and repository depth is studied. Results relative to the temperature increase are close to those of the in-room option.

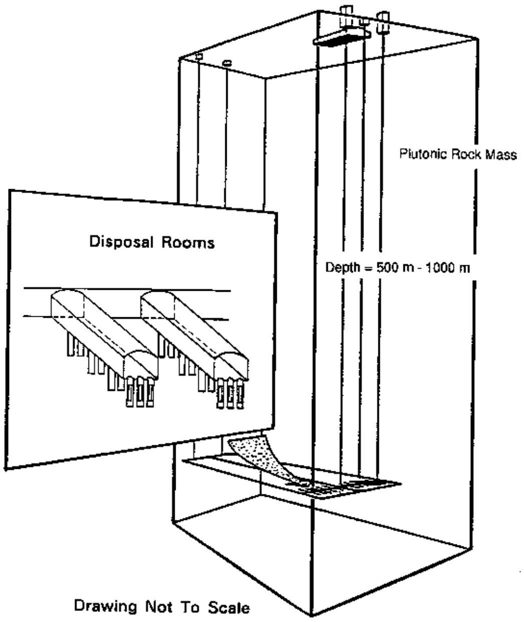
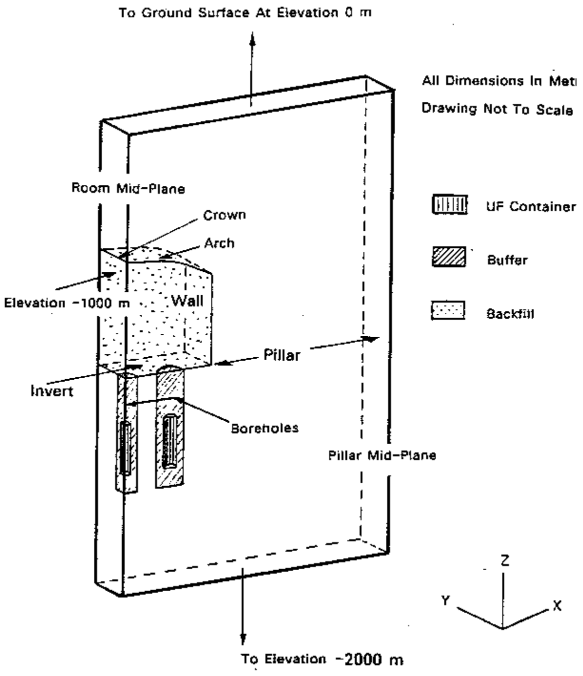


Figure 6: Schematic illustration of the Canadian concept of a nuclear fuel waste disposal vault with the boreholes emplacement option (from[129])



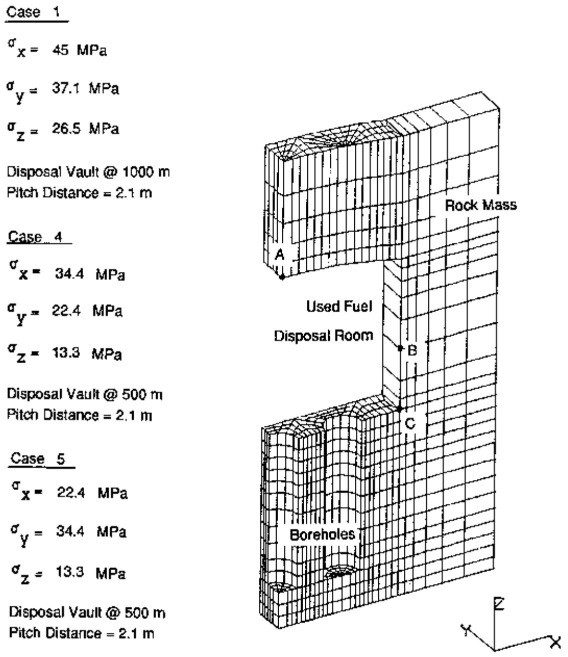


Figure 7: Perspective view of a unit cell in

Figure 8: Finite element discretization of the

the near-field of a disposal vault (from[129])

central part of the unit cell (from[129])

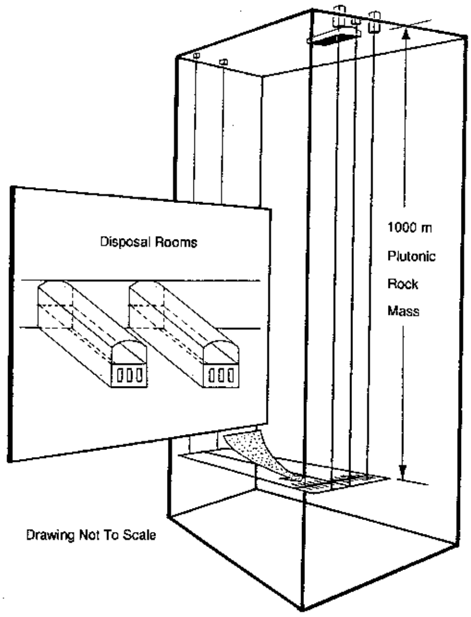


Figure 9: Schematic illustration of the Canadian concept of a nuclear fuel waste disposal vault with the in-room emplacement option (from[130])

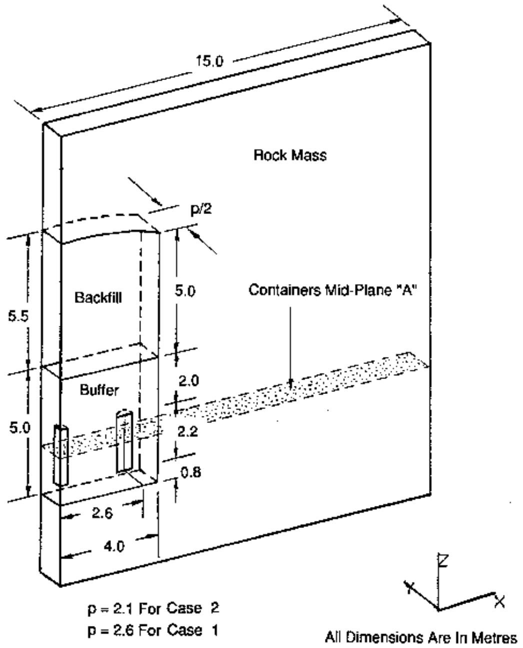


Figure 10: Dimensions of a unit cell for the in-room emplacement option (from[130])

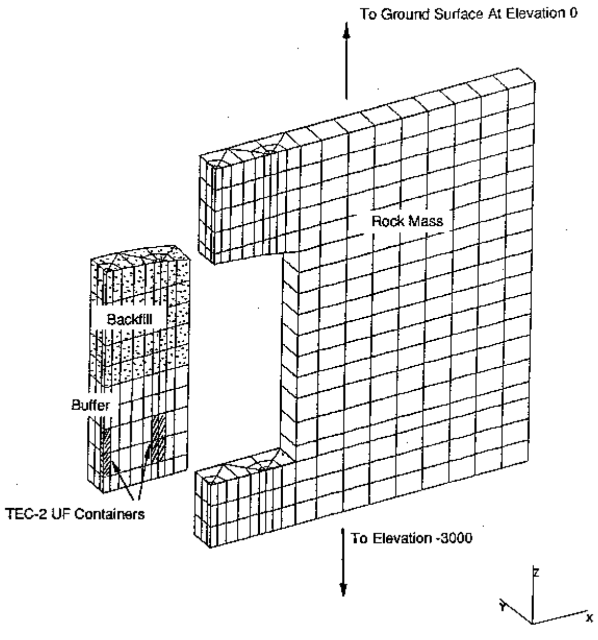


Figure 11: Finite element discretization of the central part of the unit cell (from[130])

4.3.2. Thermal modelling of the Whiteshell area

The work reported in ref. [27] is a detailed, site-specific modelling exercise, of which thermal calculations are only a small part. The disposal concept involves a network of horizontal tunnels and galleries at a depth of 500 to 1,000 m in the Canadian shield. The containers are to be buried according to the in-room or borehole schemes discussed in the previous section. However, unlike the previously discussed studies, this work uses a less detailed near-field representation and focuses on the modification of the local and regional flow field.

All modelling is based on the Equivalent Porous Medium concept, where major fracture zones are explicitly taken into account. Calculations are made with the Finite-Element code MOTIF. The rock mass is structured in 5 homogeneous layers where permeability as well as porosity decrease with depth (respectively from 10^{-15}m^2 to 10^{-21}m^2 and from 0.005 to 0.003). Permeability is anisotropic in the two top layers, with a vertical value 5 times higher than the horizontal one. Major fracture zones are explicitly represented as porous media with a thickness of 20 m and a permeability two to six orders of magnitude higher than that of the surrounding rock and a porosity 1.6 to 33 times higher.

Thermal parameters are as follows: thermal conductivity of the rock: 3.34 W/m^{o}C; specific heat: 800 J/(kg^{o}C); rock density: 2640 kg/m^3. An anisotropic dispersivity tensor is included: 6 m for the longitudinal dispersivity, 0.6 m for the transverse dispersivity. For non-isothermal fluid flow, water density depends on temperature (quadratic law) and on pressure (linear law).

The concept of a waste-exclusion zone is used to characterise the region extending horizontally from the side of the waste-emplacement area closest to a fracture zone up to the fracture zone.

First, a two-dimensional model is developed : a 27 km × 4 km cross-section corresponding approximately to a groundwater flow line. Thermal boundary conditions are prescribed temperatures, according to a geothermal gradient of 11.5 ^{o}C/km, and a surface temperature of 6 ^{o}C. The repository is represented as a line source at a depth of 500 m with a thermal output of 11.6 W/m^2. The maximum perturbation of the flow by temperature occurs around 10,000 years. The water velocity is increased by, at most, a factor of 10 close to the vault, but this effect decreases rapidly with distance. The maximum velocity increase in fracture zones is about 75 %. No formation of convection cells is shown to occur (remember that the permeability at the repository level is about 10^{-12}m/s). The travel times from the vault to the surface vary from 890 years to 2.4 10^7 years. These values do not to any great extent depend on the thermal effect : the shortest travel times vary between 1,600 years (no thermal effect) to 1,300 years (geothermal gradient only) and 890 years (thermal source term). The influence on the longest travel times is negligible, because in the regions that contribute most to the transfer times, there is no temperature change.

The three-dimensional approach starts with a regional model covering the whole Whiteshell Research Area, down to a depth of 4 km. A local model is then derived on a refined mesh with boundary conditions extracted from the regional model. The local model covers 10 km × 9 km and extends to a depth of 1.5 km. The Finite-Element mesh contains 15,144 elements and 16,944 nodes. The thermal boundary conditions are the same as in the 2-D model. The heat source is uniformly spread over a plane. The results of the thermal calculations are very close to those of the 2-D model: the maximum temperature increase is 72 ^{o}C after 8,800 years and drops back to zero after about 100,000 years. Water velocities in the fracture zones are increased by, at most, 50 % due to thermal effects. In sparsely fractured zones, where the velocities are about 3 orders of magnitude lower, an increase by one order of magnitude is found. Close to the vault, the maximum increase is by 30 times, and the average increase is 100 % after 2,000 years. The velocity direction may be inverted locally, but the average angular deviation is only 15^{o}. Far from the vault (at a distance of 1 km), the maximum increase in velocity is again by a factor of 30, but the average increase is only 50 %. The maximum angular deviation is 145^{o}. No convection cells are found to occur in fractures. The maximum reduction in travel times is about 24 %. Globally, the average reduction in convection times is 25 %. The largest reduction is 50 %.

The conclusions of the thermal aspect of this work are quoted directly from the report:

"Although the vault heating causes a large perturbation in the groundwater velocity near the hypothetical vault which lasts as long as 100,000 years, the majority of the convective transport paths leading from the vault to discharge locations at the surface are not significantly affected by the vault heat. The reason is that the movement of groundwater through the sparsely-fractured rock is usually so slow that the convective travel time from the vault to the surface is generally much longer than the duration of the velocity perturbation.

Thermal convection in the groundwater flow field surrounding the vault, due to heat generated by the fuel waste in the vault, may or may not be important depending upon the size of the waste-exclusion distance. For a 46 m waste-exclusion distance, thermal convection due to waste heat does not significantly affect the overall groundwater travel time from the vault to the surface. For a 10 m exclusion distance and for no waste-exclusion zone, there is some effect and this results in reduced travel times".

Parameter	Value	reference
Thermal conductivity of granite	3 W/m/^{o}C	[129],[130]
Thermal conductivity of buffer	1.5 W/m/^{o}C	[129],[130]
Thermal conductivity of backfill	1.5 W/m/^{o}C	[129],[130]
Thermal conductivity of container	1.5 W/m/^{o}C	[129],[130]
Thermal conductivity of granite	3.34 W/m/^{o}C	[27]
Specific heat of granite	845 J/kg/^{o}C	[129],[130]
Specific heat of buffer & backfill	750 J/kg/^{o}C	[129],[130]
Specific heat of container	500 J/kg/^{o}C	[129],[130]
Specific heat of granite	800 J/kg/^{o}C	[27]
Density of granite	2650 kg/m^3	[129],[130]
Density of granite	2640 kg/m^3	[27]
Density of buffer	1670 kg/m^3	[129],[130]
Density of backfill	2100 kg/m^3	[129],[130]
Density of container	39800 kg/m^3	[129],[130]

Table 3: Parameter values used in the Canadian studies (values in parentheses indicate ranges of variation)

4.4. United Kingdom

The United Kingdom has provided some pioneering contributions on the subject of thermal effects in crystalline media. This is reflected in the work by the Harwell group, from which we have extracted a few representative examples. The emphasis is nowadays more on the design of a ILW repository with possible applications to some aspects of HLW management ([96]).

Bourke (ref.[21]) shows a very early approach to the problem of thermal loading. With an initial output of 10 kW per waste container, a temperature rise of the order of 1,000^{o}C is considered, with a probability of melting of the rock as well as of the waste package. Corrective measures are proposed in terms of initial cooling and “waste dispersion”.

In Hodgkinson ([65]), temperature evaluations are based on a less drastic heat production, obtained through an appropriate combination of initial cooling and waste package spacing. A simplified model of the heat source is used: heat is uniformly released over a spherical volume. This allows an analytical solution of the heat transfer equation to be developed.

The same modelling approach is used in Beale et al. ([12]) to represent the following set-up: the containers have a length of 3 metres and an initial thermal output of 1 kW. They are arranged in a cubic set-up, aimed at minimising the length of the galleries, and based on a postulated higher probability of finding a continuously sound rock mass in the vertical than in the horizontal direction. Thermal parameters for the granite are taken from an in-situ heating experiment on a Cornish granite, performed on a 5 m scale: the thermal conductivity is 4 W/m^{o}C and the specific heat 2.1 MJ/m^{3} ^{o}C.

Hodgkinson ([66]) presents calculations to assess the influence of buoyancy flow on the transfer of radionuclides. The fractured medium is treated as an equivalent continuous medium, in which the flow is Darcian. Heat transfer is by conduction only. As in the previous references, a hypothesis of axial symmetry is used, and the heat source is treated as uniformly spread throughout a sphere. Thus, an analytical approach is possible to temperature as well as to pressure and stream functions. A regional gradient is superimposed in some examples. This study shows the possibility of flow paths to the surface being established due to density effects, with travel times on the order of a few hundred to a few thousand years (see fig. *12*).

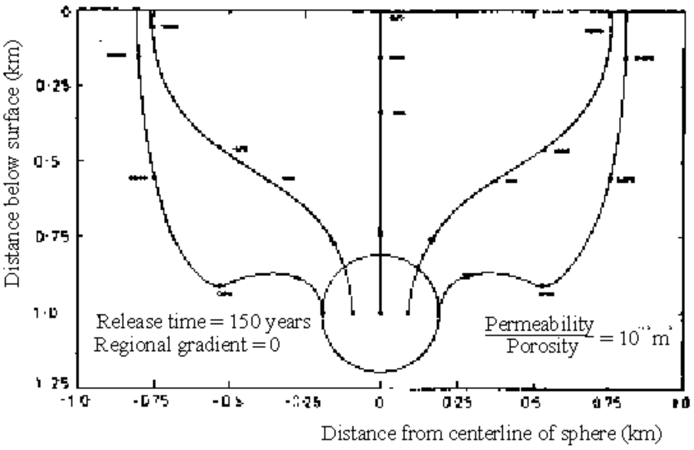


Figure 12: Thermal pathlines (from[66]*)*

In Bourke and Robinson ([22]), the same approach is extended to compare the transit times associated with natural water circulation to those due to buoyancy flow. The results are of a generic nature and highly dependent on hypotheses made on the parameters, but the general conclusion is that thermally driven flow will dominate over natural flow for several thousand years. The effects of repository geometry and depth as well as of cooling time are studied. The possibility and consequences of a thermal load associated with ILW is also considered.

Parameter	Value	reference
Thermal conductivity of granite	4 W/m/^{o}C	[12]
Specific heat of granite	2.1 MJ/m^{3}/^{o}C	[12]

Table 4: Parameter values used in British studies

4.5. France

4.5.1. CCE “Thermal-loading” study

This study (ref.[24]) may be considered as the first French effort to model the conditions around a realistic repository. The emphasis of the study is on the effects of thermal loading, and on the maximum load admissible in order to maintain these effects at an acceptable level. The study covers three types of geological formations: clay, granite and salt. Below, we briefly review the approach and the results obtained for granite.

The exercise aims at simulating a realistic geometry, based on a design study. The depth of the repository is 1,000 m. It includes 82 galleries, each 2,300 m long, and separated by 26-m intervals. 100 m deep boreholes, 30 m apart, contain 5 canisters each. The initial heat release is close to 990 W per canister. This arrangement leads to an average load of 5.8 W/m^2. The influence of the buffer material properties is studied at the local scale. In global calculations, the buffer is assumed to have the same thermal properties as the granite.

Thermal parameters have the following values: 2.5 W/m^oC for thermal conductivity and 2.2 $MJ/m^3\ ^oC$ for specific heat. These parameters result from a compilation of values obtained in the US, UKAEA, Stripa, and at various Far-Eastern and French sites. A weak variation of these properties with temperature is mentioned, but viewed as negligible in the range of the obtained temperatures.

Two modelling scales are considered: local (temperature distribution near the canisters) and global (granitic formation).

The local-scale calculations are done in two stages: first, an axisymmetric Finite-Element model computes the effect of a single container, situated near the centre of the repository. In the second stage, the influences of each elementary source are summed. This allows the effect of the borehole spacing and the rate at which containers are put in place to be investigated.

The global-scale model is based on an axisymmetric approximation: the repository is represented as a homogeneous disk with a thickness of 100 m and a radius of 1,300 m, in which the heat is homogeneously released. This model uses a Finite-Element code based on a quadratic spatial approximation.

Two other aspects of the project are worth mentioning:

- Coupled heat transfer and water flow are modelled for a simplified geometry in which major vertical fracture zones are explicitly taken into account. It is shown that the development of the temperature field is not influenced by thermal convection. However, the density-driven flow can, in some cases, lead to short travel times for water to reach the surface (a similar analysis is made in [66], with an Equivalent Continuous Medium approach).
- The possibility of coupling heat transfer with mass transfer (Soret effect) is studied on a bibliographical basis.

4.5.2. « Vie d'un Site » - " Life of a site " - study

Phases I and II of this series of three studies (ref.[51], [52], [39]) were carried out in the framework of a shared cost action between the EEC (MIRAGE project) and the French Commissariat for Atomic Energy (CEA) and Phase III under contract with the CEA. Its purpose is to use data from a French granitic site (Auriat site) for a methodological simulation exercise of a nuclear waste disposal facility. Phase I deals with hydrological aspects, while Phases II and III are specifically devoted to the evaluation of heat transfer due to the thermal loading.

The general geological framework is that of the Auriat Site, situated in central France. The modelled area is a vertical cross-section with a horizontal extent of 13 km, and a vertical one of around 2,500 m. This cross-section covers the major recharge zones and outlets of the rock mass. The fractured medium is treated as an Equivalent Continuous Medium in Phases I and II, while regional fracture zones are explicitly introduced in Phase III. Coupled flow and heat movement is represented. The corresponding equations are solved by the Finite-Element technique (METIS code).

The heat source is uniformly released into the entire volume containing the repository. Three possible repository geometries are considered, representing a more or less compact set-up of the canisters, associated with different periods of preliminary storage.

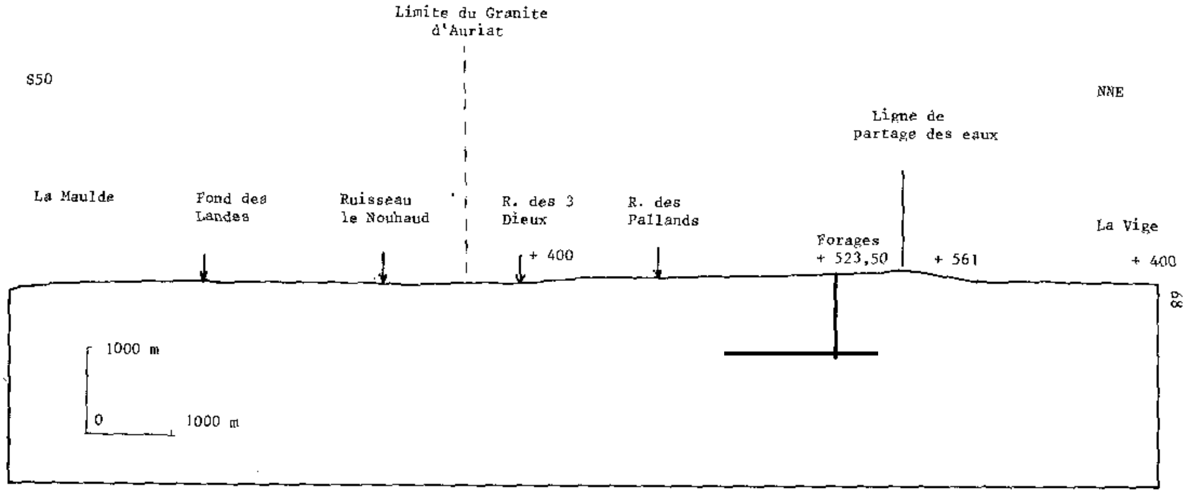


Figure 13: Cross section of the Auriat site (from[51]*)*

Results of Phase II: For the reference values of the parameters as well as for realistic variations, the heat transfer is shown to be independent of the flow, which in turn is weakly modified by the temperature rise. The thermal phase extends over a period of approximately 10,000 years. The averaged source is compared to a more precise local model of heat release around a borehole. The discrepancy between the two models vanishes after 100 years. An optimum discretization of the repository zone is defined by comparison with analytical solutions. The influence of 2-D as compared to that of 3-D modelling is studied. 2-D modelling appears sufficient as long as there is no need for a detailed description of the near-field temperature. Finally, the continuous medium is compared to a double-medium model describing the role of fractures. The continuous model is shown to be satisfactory for the range of parameters characteristic of the Auriat site.

Results of Phase III: The purpose of this phase is to extend the hypotheses of Phase II and to assess more thoroughly the validity domain of its conclusions. The following aspects are studied: variation of the regional hydraulic conductivity by two orders of magnitude; introduction of large-scale fracture zones and modification of the boundary conditions. The general conclusion of this phase is that, in all cases, heat transfer remains controlled by pure conduction. The influence of heat on the flow is limited and never leads to convection. This result, which is contradictory to the results of section 4.5.1, is discussed in section 5.1.

4.5.3. PAGIS study

Although this CEC study is a joint effort by Belgium, Germany, France and the United Kingdom, it is discussed here because the part devoted to granite is entirely French.

The 6-year PAGIS project (1982-1988) was started by the CEC in order to improve the methodology of modelling a repository site by using real data whenever possible. The disposal options considered are clay, granite, salt and sub-seabed.

For granitic formations, three typical sites were considered:

- The French site of Auriat, representing an intrusive granite rock mass
- The French site of Barfleur, characteristic of a coastal environment.
- A notional site describing a granite mass covered by a thick sedimentary layer (“British site”).

The repository depth is between 500 and 1,000 m at the Auriat site, 500 m at the Barfleur site and 980 m at the British site.

The repository design is common to the three sites. It consists of a single level of galleries. Vertical boreholes receive the canisters. Two designs are considered, each one with a different cooling time before the emplacement of the waste: for a 30-year cooling time, 1,800 boreholes are used, each containing 20 canisters. The total area of the repository is 1,500 m X 1,500 m. For a 100-year cooling period, a more compact design is possible: each borehole contains three stacks of 20 containers. The total area is then 600 m X 600 m.

Thermal modelling is approached as in the "thermal loading" study (section 4.5.1): local-scale calculations are done in two stages. First, an axisymmetric Finite-Element model is used to compute the effect of a single container, situated near the centre of the repository. In the second stage, the influences attributable to each elementary source are summed. In this manner, it is possible to investigate the effect of different borehole arrangements. The global- scale model is based on an axisymmetric approximation: the repository is represented as a homogeneous disk, into which the heat is homogeneously released.

Thermal parameters include thermal conductivity for granite, measured on three different samples of the Auriat granite: values of 3.19 W/m^{o}C, 3.56 W/m^{o}C and 2.98 W/m^{o}C were found. Values for the heat capacity vary between 650 J/Kg^{o}C and 1,400 J/Kg^{o}C, with an average of 700 J/Kg^{o}C. The value of the thermal conductivity in the buffer material is also discussed: a range of 0.8 to 1.1 W/m^{o}C is given for dry bentonite, and 1.35 to 1.45 W/m^{o}C for wet bentonite. The possibility of increasing the dry conductivity by including sand, crushed granite or even metallic compounds is mentioned.

The bentonite resaturation time is evaluated with a simple sharp-front model. A typical value of 8 months is found, and an upper limit, taking into account parameter uncertainty, of a few tens of years.

Finally, climate aspects are briefly discussed from a qualitative standpoint: possible types of climatic evolution of the three sites are discussed in view of their past history. However, this aspect is not taken into account in the calculations.

Parameter	Value	reference
Thermal conductivity of granite	2.5 W/m/^{o}C	[24]
Thermal conductivity of granite	2.98; 3.19; 3.56 W/m/^{o}C	[132]
Thermal conductivity of bentonite	0.8 – 1.1 W/m/^{o}C	[132], dry conditions
Thermal conductivity of bentonite	1.35 – 1.45 W/m/^{o}C	[132], wet conditions
Specific heat of granite	2.2 MJ/m^3/^{o}C	[24]
Specific heat of granite	700 J/kg/^{o}C (650 – 1400)	[132]

Table 5: Parameter values used in French studies (values in parentheses indicate ranges of variation)

5. Modelling issues

5.1. Thermoconvection

The coupling between flow and heat transfer in terms of density-driven flow is discussed in a number of references. Early contributions are often based on the Equivalent Porous Medium approach. For instance, Hodgkinson, in [66], considers a spherical source. The axial symmetry of the problem allows an analytical treatment of heat transfer as well as of stream functions. A regional gradient is also superimposed.

Bourke and Robinson [22]) compare the density-driven flow with the natural flow in the same type of geometry.

In Runchal and Maini ([111]), a vertical cross-section is considered. The source term is distributed uniformly over a horizontal rectangle. The rock has a stratified permeability. A discretized approach is used to solve the coupled equations of flow and heat transfer. A regional gradient is imposed. For a regional hydraulic conductivity of 5 10^{-10}m/s, large convection cells are shown to form and last for several thousand years, with recirculation of water through the repository.

In Wang et al. ([136]), the source term is approximated by a disk. A detailed study is made of the influence of waste type, cooling period, repository size, thermal properties of the rock. Buyoancy effects are shown on a very schematic fracture geometry consisting of a horizontal fracture connecting a recharge and a discharge zone, and of a vertical conduit over the repository. Heat transfer as well as flow are solved analytically.

Wang and Tsang ([135]) start from the same thermal model and analyse the density effects on a set of two vertical fractures, one crossing the repository centre, the other perpendicular and at a varying distance from the repository.

Generally, the above-mentioned studies show that the flow due to buoyancy can dominate the natural flow for several thousand years. It is also shown that thermal transfer is dominated by conduction, and that the effect of the convective flux is negligible. Studies by Goblet ([52]) and Dewiere and Goblet ([39]), also based on the equivalent continuous approach with explicit representation of major regional fractures, show that for the permeability values measured on the French site at Auriat (of the order of 10^{-12}m/s), the influence of heat on the hydraulic pattern is very small, and does not lead to the formation of convection cells. The second study also shows that the surface boundary condition has an important influence on the buoyancy-driven flow: whereas there is a noticeable flow perturbation for a uniform regional gradient, such as the one used e.g. by Runchal and Maini, this effect becomes negligible when regional flow is driven by an uneven topography as is the case on the Auriat site. Associated transit times are, in any case, much greater than in the Runchal and Maini study, due to a ten times smaller thermal load, closer to values considered nowadays.

A general conclusion by all the authors is that the occurrence and geometry of density-driven flow is highly dependent on local conditions (heterogeneity of the medium, boundary conditions, etc).

A more specific representation of the fractured medium is proposed in some references. For instance, Murphy ([94]) analyses in a theoretical way the onset of natural convective instabilities in vertical fractures. He demonstrates the possibility of a cyclic behaviour with alternating phases of convective cells and immobility. Hozanski, in [24], models the impact of a repository on water movement in a set of parallel fractures.
A site-specific study of density-driven flow in the Whiteshell research area (Canada) is discussed in section 4.3.2.

5.2. Dimensionality

It appears that, generally, except for small-scale laboratory experiments, 2- and 3-D models are the rule. 2-D models are well adapted to vertical cross-sections or to axially symmetric systems. With these models the influence of coupled mechanisms can be shown whereas they are difficult to model in 3 dimensions. However, the phenomenology of coupling in 3 dimensions is more subtle than what 2-D models can represent: for instance, density coupling leads to different flow patterns in a three-dimensional situation (annular cells in a plane layer) and in a two-dimensional situation, with different stability conditions. Likewise, one must take particular care when models explicitly include fractures, because the inherent hypothesis that the fractures are perpendicular to the model plane is very restrictive.

The local-scale description of complex mechanisms such as the water saturation state of buffers seldom seems to be tackled in more than 2-D. Hypotheses regarding the axial symmetry of the system are generally used.

In detailed modelling of the near-field behaviour, including the heterogeneity of materials (buffer, air gaps, canister, host rock, etc.), the choice of a 3-D approach is increasingly frequent. In view of the presently available computing resources, this restricts the size of the modelled domain. Symmetry assumptions are generally used to limit the domain, or boundary conditions are inferred from a large-scale domain. The discretization is sometimes very detailed (down to 1 cm to model air gaps, for instance).

Note that the exponentially increasing power of computers will probably in the near future extend the capabilities of 3-D approaches to a much larger scale. However, this prospect should not cause exaggerated optimism, since the parameters required for full-scale 3-D modelling will always be very difficult to acquire. Ref. [27] shows a good example of 3D analysis for a site model.

5.3. Non linear phenomena

In a description of coupled thermo-hydro-mechanical mechanisms, non linearity is the general rule. When one is interested only in temperature calculations, however, the situation is much more favourable: it seems as if the non linearity related to the variation of thermal parameters with temperature is unimportant. The main source of non linearity is related to the variation in water content of the buffer material. This mechanism is not easy to represent, but its influence on temperature fields is limited. Validation experiments such as the FEBEX program, the Big Ben experiment or the Kamaishi Mine heating experiment, are of a crucial importance in this field.

5.4. Source description

Judging by the references, the description of the thermal output of the waste is very similar in all European countries. This is due to similar choices regarding the cooling period and the general repository design (distance between boreholes).

The case of MOX fuel is special: ref. [50] discusses the thermal output in three different management options:

- No reprocessing
- Reprocessing of UOX fuel only
- Reprocessing of UOX and MOX fuel.

The heat output is very different in individual fuel assemblies or waste packages: a MOX fuel assembly emits from 2 to 6 times more power than a UOX assembly. The power also decreases more slowly. A (UOX + MOX) waste package emits 1.5 to 4 times more heat than a UOX package, and the heat power also decreases more slowly. However, when one looks at the total power for given assumptions regarding the inventory, the difference is less striking: the produced heat is about the same after 35 years out of the reactor. Afterwards, the decrease is fastest for maximum reprocessing, with a difference of 27 % after 100 years and 34 % after 300 years.

6. Experimental support for parameter evaluation

6.1. Börgesson et al. (1994, SKB TR 94-29)

This work deals with the heat conductivity of a bentonite-type material. Several important aspects are discussed in this study :

- theoretical models of the variation of the conductivity with water saturation, void ratio, temperature and pressure
- laboratory measurements based on the injection of a thermal pulse and detailed discussion of this technique, leading to a set of recommendations regarding the experimental procedure
- conduction values inferred from field tests.

The general conclusion from this extensive compilation is that the values of heat conductivity in bentonite can be predicted with a reasonable degree of precision as a function of porosity and water content. Laboratory and field values are consistent : no noticeable scale effect appears ; this is not totally surprising because the size of the bentonite structure surrounding a canister is not much larger than that of the laboratory samples.

The heat conductivity of buffers with a low water content is more difficult to predict, because of the complex effect of vapour redistribution.
The residual uncertainty demonstrated by this study should be put in perspective by calculating its impact on temperature distribution around a canister.

6.2. Stripa

Heater tests performed in Stripa are reported in [34]: 3 types of heater tests were carried out in 1978 at a depth of 340 m: the first involved an array of 8 electric heaters, scaled so as to simulate in one year the heat conduction field around radioactive waste canisters over a period of a decade. The second and third tests involved a single heater, 0.3 m in diameter and 3 m in length, buried in a vertical hole (0.406 × 5.5 m) drilled from the floor of a drift. The heater delivered a power of 3.6 kW in the second test, corresponding to a canister of High-Level Waste 5 years out of the reactor, and 5 kW in the third test (canister 3 years out of the reactor).

Experiments 2 and 3 are modelled in a simple way in [34], demonstrating that heat propagation is essentially by conduction in test 2, with a possible additional contribution of convection in test 3, and that phase change from water to steam does not play a significant role, although a temperature of over 100^{o}C is reached in the third test.

6.3. Fanay-Augères

The French experiment at Fanay-Augères was set up by the IPSN in the framework of a shared-cost action with the European Community. The experiment was proposed as a test case in the DECOVALEX I project. This section deals with the description of the experimental aspects and the modelling carried out in the framework of the programme. The comparative aspects of the modelling are discussed in the DECOVALEX section (7).

Experiment description

The Fanay-Augères site is an abandoned uranium mine in central France ([38]). It has been used for various experimental programmes concerned with the hydraulic behaviour of fractured rock masses. The experiment in question was performed between 1987 and 1988, and concerned the emplacement of a heating element in an experimental room and the subsequent monitoring of temperature and deformations (the medium is partially desaturated which prevents hydraulic measurements).

The experimental site consists of a 12 x 10 x 5 m room at a depth of 100 m accessed by a gallery. The heating source is composed of 5 elements, each 1.5 m long and 0.146 m in diameter, disposed in a quasi-horizontal plane, separated by a distance of 0.30 m. The average source position is 3 m under the floor of the experimental room. The heat output is 1 kW (200 W per element).

The heating experiment consisted of a heating phase (52 days) followed by a cooling phase (73 days). Temperature was monitored at 79 locations.
The values of thermal parameters, measured on samples, were 2.13 W/m/^{o}C for the conductivity at 20 ^{o}C, 1.95 W/m/^{o}C at 80 ^{o}C, and 2.11 MJ/m^3 ^{o}C for the heat capacity.
The experimental results are described in [38]. The maximum temperature reached by the heaters was 75^{o}C. The maximum temperature on the experimental-room floor was 14.2^{o}C, and 18°C one meter below the floor.

Modelling

The experiment was modelled by the Ecole des Mines de Paris (Centre de Géotechnique et d'Exploitation du Sous-sol) using Finite-Element simulation codes ([80], [108],[109], [110]). Two approaches were followed: first, with a two-dimensional model in radial symmetry, with a simplified representation of the source as a uniformly heated disk. This model showed a qualitative agreement between the temperatures and the measurements, but a quantitative discrepancy, especially regarding the temperature close to the heater (10^{o}C). A more refined three-dimensional model was built, with a detailed description of the source term. This model represents a noticeable improvement, but the simulated temperatures still exceed the measuremed ones. The authors explain this as a scale effect on the thermal parameters, possibly related to the fracturation of the medium. This scale effect would lead to in-situ parameter values 40% greater than those found in the laboratory.

Parameter	Value	reference
Thermal conductivity of granite	2.13 W/m/°C at 20 °C	[38]
Thermal conductivity of granite	1.95 W/m/°C at 80 °C	[38]
Specific heat of granite	2.11 MJ/m^3/°C	[38]

Table 6: Parameter values on the French site of Fanay-Augères

6.4. Grimsel: Swiss heating experiment

This experiment is described in section 4.2.3.

6.5. URL (heated rock failure tests)

This experimental program is presented in [92]. It aims at testing the integrity of a granite block subjected to heating. We present the main features of the experiment, and some modelling work.

The experiment was set up in the Canadian URL. Several 600 mm diameter observation boreholes were drilled from the floor of an experimental gallery situated at a depth of 420 m in the URL. The temperature in the granite surrounding the boreholes was raised by electric heaters situated at a distance from the boreholes on the order of a metre.

Three stages are presented in ref. [92]:

- in stage 1, one borehole was drilled and the rock was subsequently heated
- in stage 2, the rock was first heated, and the observation borehole drilled afterwards
- in stage 3, two boreholes were drilled at a short distance from each other, and the rock was heated afterwards.

In all cases, the measurement devices included thermistors, piezometers, extensometers, convergence pins, radial strain cells, thermocouples and acoustic-event sensors. In case 1, the temperature in the observation hole was raised to 85°C.

An axisymmetric numerical model satisfactorily reproduced this temperature history.

The most interesting part of the project, which is beyond the scope of this review, is the analysis of rock failure by visual as well as acoustic techniques.

6.6. FEBEX program

The FEBEX project ([43],[45],[47],[48],[69],[70],[71],[113],[133]) is of great interest and relevance for the Swedish concept for many reasons :

- the host rock is crystalline
- a bentonite buffer material is used between the canister and the rock
- expected temperatures in the near-field are in the same range as that assumed in Sweden

For these reasons, we shall review in some detail the characteristics of this project, especially as regards thermal modelling, and preliminary results.
The FEBEX (Full-scale Engineered Barriers Experiment) is predicted to last approximately seven years (1994 through 2001). Its basic purpose (ENRESA, 1998) is to demonstrate the feasibility of an EBS made of bentonite in a crystalline context, and to study the thermo-hydro-mechanical as well as the thermo-hydro-geochemical processes in the near field.

The project includes three aspects : a real-scale in-situ heater test, performed in the Swiss underground laboratory at Grimsel, an almost full-scale mock-up test performed at CIEMAT (Madrid) and various supporting laboratory experiments.

6.6.1. Description of the in-situ experiment ([45])

The in-situ test is made in a predominantly granitic rock mass at a depth of 400 m. In a 70 m long horizontal drift, a 17 m long section is isolated. The gallery diameter is 2.28 m. A set of two heaters has been installed horizontally in the drift. This differs from the Swedish concept, where the containers are placed in vertical boreholes drilled from a main gallery. The heaters reproduce the dimensions of the Swiss container : 4.54 m in length and 0.90 m in diameter. They are aligned along the axis of the gallery, inside a steel liner and surrounded by a buffer of bentonite (Ca-bentonite with a dry density of 1,700 kg/m^3). Heating started in February 1997, with a variable power input : 1,200 W per heater for 20 days, then 2,000 W per heater for another 32 days. Since then, the power has been regulated in order to achieve a maximum temperature of 100 ^{o}C at the heater-bentonite contact (power output around 2,500 W per heater).

A set of 600 measurement points provide information on temperature (189 thermocouples), humidity (159 measurements), stress, pressure, displacement and pore pressure. These measurement points are spread throughout the host rock, the clay barrier and the heaters. Gas formation is also monitored.

6.6.2. Description of the mock-up test

The mock-up test reproduces the conditions of the *in-situ* test, but at a slightly reduced scale, and in the strictly controlled conditions of a laboratory. The overall dimensions of the buffer mass are 6 m in length and 1.61 m in diameter. Two heaters are used, each one with a length of 6 m and a diameter of 0.34 m. The buffer material has a dry density of 1,750 kg/m^3, and an initial moisture content of 14 %. A hydration system provides water to moisten the bentonite mass under constant and controlled pressure. The same variables as in the in situ-test are measured at 400 points.

6.6.3. Laboratory measurements

The aim of the associated laboratory programme is to characterise the materials used in the experiment and to analyse the thermo-hydro-mechanical as well as thermo-hydro-chemical behaviour of the bentonite. Of particular interest are: the measurements of the thermal conductivity of the bentonite as a function of its water content, of the thermal conductivity of the rock and of the specific heat of the bentonite and the rock

6.6.4. Lessons from the preliminary modelling

The mock-up test was modelled *a priori*. A parametric study made it possible to examine the effects on the observed variables of some selected parameters.
The results of the base case indicate that the barrier does not reach total saturation after three years of hydration and heating. Nevertheless, the parametric studies suggest that this result is very sensitive to the parameters adopted for the retention curve and the permeability of the bentonite.

The effects of an initial flooding phase were examined. With the chosen parameters total closure of the joints was obtained before the initiation of the heating, and no other significant effect of the initial flooding was observed.

It is felt that the questions regarding the heterogeneity and the presence of discontinuities in the barrier must be carefully investigated.

6.7. Big Ben experiment

The purpose of this experiment performed at Tokai Works, Power Reactor and Nuclear Fuel Development Corporation (PNC, Japan) is to investigate the behaviour of an engineered barrier under the effect of a thermal load. The scale of the experiment is representative of the environment of a canister in a repository.

A cylinder of reinforced concrete, 6 m in diameter and 5 m high, is located under the floor of an experimental room. A central pit, 1.7 m in diameter and 4.5 m high, simulates a deposition borehole. A cylindrical heater, 1 m in diameter and 2 m high, is placed in the pit and surrounded by bentonite. All gaps are filled with quartz sand.

The power output of the heater is 0.8 kW, producing a temperature of less than 100^{o}C in the bentonite. Measurement devices include 139 temperature sensors, 8 heat-flux meters, 38 humidity sensors, besides measurements related to the mechanical response. The thermal properties of the bentonite are expressed as:
$0.33+0.031\theta$ (thermal conductivity in W/m ^{o}C)
$(100+4.2\omega)/(100+\omega)$ (specific heat in kJ/kg ^{o}C).

Temperature profiles are obtained at various dates during the 5 month long experiment. The water content is measured on samples at the end of the experiment.

The modelling of the Big Ben experiment in the framework of the DECOVALEX project is described in section 7.1.5.

Parameter	Value	reference
Thermal conductivity of bentonite	$0.33+0.031\ \theta$ (W/m/^{o}C)	[46]
Specific heat of bentonite	$(100+4.2\omega)/(100+\omega)$ (kJ/kg ^{o}C).	[46]

Table 7: Parameter values for the Big Ben experiment (q: volumetric water content; w: porosity)

6.8. Research Programmes in the HADES lab

A number of experimental programmes are conducted in the Belgian underground laboratory at Mol. This laboratory is situated in the Boom clay formation, and specifically devoted to the study of clay formations. As such, it is not directly relevant to the Swedish situation. Nevertheless, we briefly present various research programmes, that can be partly applied to a different host rock.

- The CACTUS programme (ChAracterisation of Clay under Thermal loading for Underground Storage, ref.[100]) aims at quantifying the hydro-thermo-mechanical couplings inside a clay formation after the emplacement of radioactive waste containers in a vertical borehole. Two thermal probes (CACTUS 1 and CACTUS 2) with a total length of 3.6 m and a diameter of 0.30 m, are buried at a depth of about 16 m below the test drift. These probes contain cylindrical heating elements with a sufficient heat output to reproduce the temperature conditions around waste containers after a 50-year cooling period. They also contain various measuring devices, among which are temperature probes, water-content measurement devices, pore-pressure probes. The CACTUS 1 probe was subjected to a succession of heating and cooling phases for a period of about 3 years. In ref. [100], a heating phase slightly longer than one year, followed by a cooling phase of 200 days, is reported for CACTUS 2. A Finite-Element model taking into account homogeneous properties for each material reproduces the temperature measurements with satisfactory precision.

- The CERBERUS project (Control Experiment with Radiation of the Belgian Repository for Underground Storage, ref. [97]) aims at simulating the near-field effects in an argillaceous environment of a Cogema HLW canister after 50 years cooling time. The experimental probe, buried in the Boom clay, contains a ^{60}Co source and two sets of 3 heating elements with a nominal power of 500 W each. A 5-year heating phase (1989-1994) with a constant power supply of 365 W per heater yielded results concerning the influence of heat and radiation on pore pressure, constraints, fluid chemistry, clay mineralogy, etc.
- The CLIPEX project (Clay Instrumentation Programme for the EXtension of an underground research laboratory, ref.[16]) aims at predicting the behaviour of the Boom clay formation during the projected extension of the laboratory. It is essentially based on the study of the mechanical response by the clay during and after construction.
- The PHEBUS project (Phenomenology of Hydrical Exchanges Between Underground atmosphere and Storage host-rock, ref. [111]) aims at characterising the hydraulic behaviour of compacted clays around a repository. It is based on a laboratory and an *in- situ* ventilation test.
- The PRACLAY project (ref. [131]) aims at demonstrating the technical feasibility of disposing high-level, long-lived vitrified waste canisters in a deep geological repository in clay. An important preliminary step is a large-scale heating experiment on a mock-up. The mock-up is a 5 m long section of backfill with a central tube. The thermal isolation from ambient air is obtained through a mineral-wool jacket. The temperature around the mock-up can also be controlled through a regulated heating device. A thermal-pulse technique is used to measure the evolution of the thermal conductivity during the hydration of the mock-up. A comparison between preliminary modelling results and measurements shows a higher influence of hydration than anticipated. This is attributed to a swelling of the backfill blocks, which may have reduced the thermal resistance between the blocks.
- The RESEAL project studies the feasibility of backfill in clay.

6.9. U.S. experiments

The context of nuclear waste isolation in the United States differs notably from the situation in European countries, because 1) the proposed hydrological situation is unsaturated media in order to reduce the effects of water circulation over the waste packages, and 2) a higher temperature is allowed near the waste to delay the return of humidity for as long as possible. For these reasons, the approaches to thermal problems are very different in the US: in particular, the possibility of two-phase flow is systematically considered, which makes the modelling much more complicated. Aspects of the behaviour of the unsaturated medium are discussed in, e.g. [4], [5], [7], [10], [53], [54], [55], [63], [89], [98].

However, one aspect is similar to the Swedish situation, i.e. the effect of fractures on water circulation. From the experimental viewpoint, the work done on the Yucca Mountain site may provide an opportunity for model testing. Of particular interest are the intermediate- to large- scale heating tests:

- The Large Block Test (LBT) is of sufficient scale (3 m × 3m × 4.5m) to allow the investigation of a representative fracture structure, yet small enough to allow control of the boundary conditions (ref. [53]): a quasi-planar heat source is created on one side through 5 parallel heaters; a uniform temperature is maintained on the opposite side by a heat exchanger; finally, the 4 sides are thermally isolated. A 220-day heating phase was initiated on February 28, 1997, followed by a 150-day power ramp-down, and a natural cooling phase. The maximum temperature reached is 140^o C. This provokes vapour flow and potentially, heat-pipe effects.
- The Single Heater Test and the Drift Scale Test are two large-scale in-situ tests designed to show the behaviour of a rock mass under the influence of repository-like coupled processes.

7. International Projects (DECOVALEX)

International projects dealing with thermal problems are discussed in various sections throughout this document. Here, the DECOVALEX I and II projects are discussed in some detail because they were specifically devoted to hydro-thermo-mechanical couplings.

7.1. DECOVALEX I

The DECOVALEX I Project (Development of Coupled Models and their Validation against Experiments in nuclear waste isolation [78], [79], [80], [83], [125]) is an international undertaking sponsored by organisations in Canada, Finland, France, Sweden, the U.K. and the US between 1992 and 1995. This project was devoted to the assessment of models decribing the coupled thermo-, hydro- and mechanical processes around a deep nuclear waste repository. The emphasis was on fractured rocks and buffer material. Temperature calculations represented only a small part of the work done within the project, but in this report we shall focus on this aspect.

The project was structured around a set of benchmarks, aimed at verifying numerical codes, and test cases based on experimental data, which provide a fairly realistic framework for verification, inter-comparison of modelling approaches and validation of models.

In this section, we discuss the lessons that can be learned from the benchmark tests and from the modelling approaches used in the test cases. The experimental aspects are discussed in section 6.

Three Benchmark Tests are relevant for granitic media: BMT 1 is a large-scale test, BMT 2 a small-scale one and BMT 3 is of intermediate scale.

Two Test Cases are related to crystalline media: TC 2 (Fanay-Augères heating experiment) and TC 3 (Big Ben experiment on buffer material).

7.1.1. Benchmark BMT 1: far-field situation

BMT 1 describes a 2-D vertical cross-section through a regional rock mass. The horizontal extent is 3,000 m, the depth 1,000 m. The repository lies at a depth of 500 m. Two perpendicular sets of discontinuities are considered, with three different spacing distances: 25 m, 50 m, 100 m.

The thermal situation is governed by the following boundary conditions: prescribed temperature at the soil surface, zero thermal flux on the vertical boundaries, and geothermal flux along the bottom boundary. The thermal loading of the source is described by an exponential time function.

Numerical techniques used on this case include Finite Elements (equivalent continuous medium approach, heat convection is not considered), Finite Elements with explicit description of fractures by 1-D ("joint") elements and without heat convection, Distinct Elements (without heat convection), and Finite Elements (equivalent continuous medium with heat convection).

The major findings of this exercise are ([85],[93]):

- Temperature-field results from different teams are in good agreement. Differences can be explained by mesh effects.
- The effect of convective flux on heat transfer seems negligible, although, on this point, two teams have reached diverging conclusions. Note that both teams use an equivalent continuum approach, which may not be the most appropriate one to quantify the convective effect around fractures.
- Fractures have no influence on heat transfer.

7.1.2. Benchmark BMT 2: Near-field model with fractures

This exercise describes a small rock block (0.75 m X 0.50 m) intersected by two vertical and two horizontal fractures.

The thermal boundary conditions are: zero flux on the top and bottom boundaries, prescribed temperature on a vertical boundary and prescribed thermal flux on a limited section of the fourth boundary.

As BMT 1, this test case was modelled using Finite Elements as well as Distinct Elements, with and without heat convection.

The main conclusions of this exercise are ([85], [26]

- A significant difference is found between the results by teams who take into account heat convection and those who do not. Note that a hydraulic gradient is prescribed across the domain, and that the modelled section is horizontal. The mechanism is therefore forced convection.
- Differences between models of each sub-class (with or without convection) are minor.

7.1.3. Benchmark BMT 3: Near-field model with a realistic fracture network

This case represents an intermediate-scale problem: vertical 50 m X 50 m cross-section, situated at a depth of 500 m below ground level. The domain is intersected by a tunnel with a deposition hole where a heat source is simulated. The rock mass is crossed by a fracture network inspired by the Stripa site (6,580 fractures).

A variety of modelling approaches are used on the problem:

- Discrete Fracture Network (no thermal modelling)
- Finite-Element solution (equivalent continuum, homogenisation on a 10- and 25 m scale)
- Distinct-Element Model with a simplified fracture network
- Finite-Difference solution (equivalent continuum, no homogenisation).

The main conclusions of this exercise are ([85]:

- Good agreement between temperature fields calculated with various techniques
- No influence of heat convection.

7.1.4. Test Case TC 2: Fanay-Augères heating experiment

The heating experiment on the French site at Fanay-Augères, described in section 6.3, was modelled with three different techniques: Distinct-Element Method, Discrete Finite-Element Method (taking discontinuities into account), and Continuous Finite-Element Method (no discontinuities). This work is reported in [108] and [80]. The salient aspects are:

- Difficulty in coping with a realistic 3-D geometry including a room, a complex heating device and a number of fractures (6 fractures were chosen for the specification of the test case). Only one team chose to represent the heaters in detail.

The typical number of nodes is around 7,000, which is rather low for a 3-D geometry.

- Thermal calculations imply a full solution of the heat equation in the Finite-Element approaches. In the Distinct-Element Method, a quasi-analytical approach is used, whereby each heater is represented by 50 point sources.
- Thermal conductivity is considered independent of temperature except in one calculation, where it depends linearly on temperature. This has no noticeable effect on temperature (this aspect was also examined in [110]).
- Computed temperatures generally agree well qualitatively. They exceed the measured temperatures, especially close to the source. This discrepancy is reduced when a more realistic representation of the source is used. This quality of representation can be obtained by Finite-Element refinement as well as by the semi-analytical approach associated with the Distinct-Element Method.
- Results close to the source show a mesh dependence in the Finite-Element calculations.

7.1.5. Test Case TC 3: Big-Ben heating experiment

The Big Ben experiment, described in section 6.7, includes two-phase flow under variable temperature. This complex phenomenology was tackled by several teams, using Finite Element codes, under various assumptions ([46], [80]):

- Evaporation-condensation process described by varying the thermal conductivity with the temperature and water content
- Gas and water flow neglected
- Unsaturated flow model.

Two laws are proposed for the variation of thermal conductivity with water content. However, the experimental results are equally well reproduced with a constant conductivity, which demonstrates the limited impact of this variation.

The calculated temperature fields are in reasonable agreement with the measured values (maximum error 5 ^{o}C). The difference between values obtained by different teams is, at most, 10 ^{o}C. The discrepancies between the different calculated values and between calculated values and measurements seem to be due mostly to different boundary conditions (heat transfer coefficients along the boundaries).

The modelling of water content is consistent among the models and agrees well with the measurements.

7.1.6. Lessons learned from DECOVALEX I

The major findings concerning temperature modelling in the DECOVALEX I project are discussed e.g. in [40], [83], [125]. To quote [83]:

“The temperature predictions made by the different approaches and computer codes for all TC or BMT problems with thermal processes involved are very consistent among themselves and in reasonable agreement with the experimental measurements. The agreement is better for fractured rocks than that for buffer materials. We may conclude that the mathematical model for the heat transport equations used in the computer codes in the DECOVALEX project is a realistic representation of the thermal process in fractured rocks and buffer materials and can be trusted to produce realistic thermal results for performance assessments of nuclear waste repositories. The minor differences observed are generally due to either differences in mesh resolution or whether thermal convection is taken into account. The latter is not expected to be significant for fractured rock systems except in the very close vicinity of the heat source."

7.2. DECOVALEX II

The DECOVALEX II project started in November 1995 as a continuation of DECOVALEX I. This project was initiated to extend the findings of DECOVALEX I to more complex and realistic *in-situ* situations (which generally implies a larger scale). The following objectives were formulated as a result of DECOVALEX I (ref. [84]):

1) validation of mathematical models and computer codes for coupled T-H-M processes by large-scale field experiments of complex and realistic initial-boundary conditions, rather than by small-scale laboratory tests with well controlled test conditions;
2) understanding the current capacities to develop computer models of real sites with incomplete data on coupled thermo-hydro-mechanical behaviour and on properties of host rock and buffer materials;
3) understanding the current state-of-the-art of the constitutive relations of rock discontinuities, which are among the most crucial and least understood factors controlling the coupled T-H-M processes in fractured rocks; and
4) reaching a consensus about the coupled thermo-hydro-mechanical processes related to design and performance assessment of underground nuclear waste repositories.

The following tasks were defined:

Task 1: Numerical study of Nirex's RCF Shaft excavation at Sellafield, UK. Simulation of the coupled hydro-mechanical processes of the RCF3 pumping test and responses of the rock mass to the shaft excavation, including study of the excavation-induced disturbed zone (EDZ). Task 2: Numerical study of PNC's in-situ THM experiments in Kamaishi Mine, Japan. An integrated investigation on a complete rock-buffer-heater system under *in-situ* conditions over a long period of time.

Task 3: Review of the state-of-the-art-of the constitutive relations of rock joints.

Task 4: A report on the current understanding of the coupled T-H-M processes and how it relates to design and performance assessment of radioactive waste repositories.

Thermal aspects are involved only in task 2 (Kamaishi mine heating experiment). Our review will therefore focus on this part.

7.2.1. Kamaishi Mine experiment

7.2.1.1.Experiment

The experiment ([81]) was carried out in a fractured rock mass, at 550 m below ground level. A test pit, 5 m deep and 1.7 m in diameter, was drilled from the floor of a 5 × 7 m alcove. The test pit was filled with bentonite and contained an electric heater, 2 m high and 1.04 m in diameter. An extensive fracture mapping was done at the floor of the test drift.

The heating capacity was 10 kW. A large number of measurement devices registered data as a function of time inside the rock mass (pore pressure, strain, relative displacement) and inside the buffer material (pore pressure, temperature, pressure, heat flux, strain, suction, water content). Finally, water was sampled at regular intervals along predefined profiles. The heating phase lasted 258 days and was followed by a cooling period up to 515 days.

A number of supporting laboratory experiments provided data for the characterisation of the bentonite:

- Suction tests: wetting and drying of 13 mm (diameter) × 9 mm (height) samples to determine the (suction-water content) curve.
- Water infiltration tests: 20 mm × 20 mm samples were submitted to an infiltration through the bottom at various temperatures, to identify the total water diffusivity (describing liquid and vapour flux of water).
- Thermal gradient tests: the water redistribution due to a prescribed thermal gradient was measured on 50 mm (diameter) × 100 mm (height) samples to determine the thermally driven water flow.
- Swelling tests: similar to the infiltration tests, but in a confined volume, to measure the stress variation induced by the variation in water content.

Other supporting measurements include, for instance, the variation of thermal conducitivity and specific heat with water content.

7.2.1.2.Modelling

The objective of Task 2C of DECOVALEX II is the modelling of the Kamaishi Mine heating experiment, i.e. (ref. [81]) “predicting the fully coupled thermo-hydro-mechanical behaviour of the complete heater-buffer-rock system at the test site, especially the interactions between different components and interfaces (heater-buffer, buffer-rock, solid-water)” and the determination of buffer properties. Two sub-tasks were identified:

- Task 2C-1: identification of the buffer properties from the laboratory experiments.
- Task 2C-2: predictive modelling of the heating experiment.

7.2.1.3.Conclusions from Task 2C

The mechanisms invoked to interpret the laboratory experiments differ somewhat between teams, e.g. regarding the driving force for vapour flow (temperature only or temperature and pressure). These differences in concept lead to slightly different parameters. As no real validation step is involved (in the sense of independent prediction of other experiments), but only a curve fitting procedure, there is no way to discriminate between the various models.

The predictive modelling of the heating experiment, using models and parameters determined from the laboratory experiments, generally show a satisfactory prediction of the temperature fields in buffer and rock, and of the water content. The prediction of pressure in the rock is generally acceptable, but the prediction of the total pressure in the buffer and displacement in the rock are not very good. This shows that one of the objectives of Task 2, predicting the interactions between different components and interfaces, requires further work.

8. Climate events

In nuclear waste repository performance assessments, changes in climate conditions are very often considered important “FEPs” (Feature, Event and Processes) that need to be considered in scenario development. Climate changes are assumed to occur both naturally, and as a potential consequence of human action, as, for example, the greenhouse effect.

In most studies, climate changes are limited to a variation with time of the rainfall pattern or the outside temperature or a change in the sea level as ice caps on the poles or continents melt or form. Changes of the outside temperature can be on the order of up to 20°C for a very significant climate change (from optimum temperature to extreme glaciation), but the net effect on a repository situated at a depth of e.g. 500 m will at most be a temperature change at repository depth of the same order of magnitude (20°C), since the time needed for the climate change to reach the repository depth of 500 m is on the order of some thousands of years.

In Sweden and in Canada, however, climate changes have for a long time been associated with the onset of a new glaciation, when an ice sheet would build up on the surface rock above the repository. Most studies of the effect of such a glaciation have therefore been done in Sweden.

In February 1991, McEwen and Marsily for SKI presented an initial assessment of the potential significance of a temperature change for a deep geological repository (ref. [90]). They assessed the available literature on climate variations in the Quaternary and concluded that the best model for predicting the future climate in Sweden was the so-called “Milankovitch theory”, which relates past recorded temperature changes (e.g. from marine sediment cores) to the variations of three parameters of the Earth’s orbit around the sun. They determined that a prediction of future temperatures could be made by adding three cyclic orbital variations with three periods : 10,000, 40,000 and 120,000 years. They produced a predicted temperature curve for the next 150,000 years, which suggested a gradual cooling with a global minimum in 60,000 years followed by warming until a new optimum was reached in 120,000 years. The maximum amplitude of the temperature variation at the surface is 20°C (from +5°C to -15°C).

To infer the resulting effect on a repository situated at a depth of 500 m, they used an analytical solution of the heat equation, assuming pure conduction in the ground, and a local natural geothermal gradient of 1°C or 3°C/km, in a granite bedrock. They used a thermal conductivity of 3 W/m^{o}C and a heat capacity of 2.10^6 J/m^3 ^{o}C. They neglected heat transport by advection and the latent heat of freezing/fusion when the water in the ground changes from water to ice or vice versa. Their solution assumes a periodic variation of the temperature at the surface and adds the three harmonics corresponding to each period. They calculated that, without a repository, the permafrost depth would reach around 600 m with the 1°C/km natural gradient and 300 m with the 3°C/km gradient. With a repository designed according to the KBS-3 specifications by Tarandi (ref. [127]), the permafrost would only reach depths of, respectively, 350 m and 200 m with the two geothermal gradients.

They then analysed the potential effects of this permafrost on the repository, mostly in terms of groundwater flow, shaft failure and bentonite buffer degradation, which are outside the scope of this report on thermal modelling.

Ahlbom et al. (ref. [2]) at SKB also studied an ice-age scenario. They reviewed a number of climate models, and concluded that a glaciation could potentially occur in about 5,000, 20,000 and 60,000 years. An interglacial period similar to the present one might occur in 75,000 or 120,000 years.

They did not attempt to calculate the temperature distribution in the ground, but produced an estimate of the extent and thickness of the ice sheet over northern Europe, based on records of the last glacial maximum, which occurred 18,000 years ago. In Sweden, this thickness would reach 2,000 to 2,500 m. They also looked at the deflection of the crust (isostasy), sea-level changes, bedrock movement and reactivation of faults, hydraulic conditions during glaciation and deglaciation, and possible changes in groundwater chemistry. They summarised their findings by giving a “reference” scenario describing the conditions that might be expected to prevail in Sweden over the next 130,000 years.

Within Site 94, King-Clayton et al. (ref. [87]) developed a “Central scenario” for SKI which included climate changes. Three deterministic climate scenarios were designed for the Äspö area, including three major glaciations in 20,000, 50,000 and 90,000 years. These glaciations differ in the following assumptions : (i) two successive ice sheets form at circa 50-70 ka and 90-110 ka, with a moderately warm-based ice; (ii) only one ice sheet forms at 50-70 ka, with moderately warm-based ice; (iii) two successive ice sheets form as in (i), but with warmer-based ice. The difference between cold-based and warm-based ice sheets was taken from the work of Boulton and Payne (ref. [20]) who modelled the development and movement of an ice sheet over the northern hemisphere, given a prescribed temperature history of the air. The two forms of temperature distribution at the base of the ice sheet were part of a modelling alternative. This model includes approximate calculations of heat exchanges between the ice sheet and the ground. To achieve a more precise modelling of the thermal consequences of these scenarios in the ground, a simple one-dimensional Finite-Difference approximation of the heat-conduction equation is used, which in some cases, includes a uniform heat source at a depth of 500 m to represent the effect of a repository. The repository design is that of KBS-3 as in Tarandi (ref. [127]). The temperature at the ground surface is derived from Boulton and Payne (ref. [20]) and prescribed for the one-dimensional model. A rock thickness of 8 km is considered, with a prescribed heat flux at the base. Contrary to McEwen and Marsily ([90]) they include in their numerical solution the latent heat of freezing/fusion, assume a rock porosity of 1%, neglect advection, and use a geothermal gradient of 14°C/km, corresponding to a natural geothermal heat flux of 42 mW/m^2, with the thermal rock properties of 3 W/m°C and $2.16x10^6$ J/m^3 °C, taken from Sundberg ([126]). The uniform heat flux produced by the waste is initially assumed to be 850 W per canister, with one canister per $150m^2$, producing an initial flux of 5.7 W/m^2. It then decays exponentially (with three imbedded exponentials), reaching values of 331 W/can at 100 years, 68 W/can at 1,000 years, and 20 W/can at 4,000 years.

The maximum temperature of 58°C at repository depth is reached a few tens of years after disposal and decays to normal values in about 120,000 years (i.e. the same temperature as if there were no repository). The residual difference between natural conditions and the presence of the repository is only of 5°C at repository depth, after 20,000 years. This temperature at repository depth is an average over 1,500 m^3 of rock surrounding the waste, and should not be considered as the peak temperature of the canister in the near field. The predicted permafrost depth at the glaciation peak (50,000 years) reaches 300 m with the repository, and 350 m without the repository. This clearly shows that even after 50,000 years, the heat output of the waste is still very significant in the ground.

The remainder of this report establishes the potential consequences of the glaciation scenario for the ice sheet geometry, rock stress, groundwater flow, groundwater chemistry and biosphere and surface conditions, which are outside the scope of this review. A detailed scenario for performance assessment is defined. Additional calculations pertinent to this scenario can be found in [61], [62], [118], [119].

In April 1996, SKI organised a “Glaciation and Hydrogeology” Workshop in Stockholm, to assemble experts on the potential impact on a repository of Climate Change and Glaciation (SKI, edited by King-Clayton et al, ref.[88]). This workshop, began by a review of climate models and continued with the hydrological, hydrochemical and tectonic aspects of glaciation. Although the proceedings contain a great deal of information, no thermal calculations are reported.

Additional discussions of glaciation can be found e.g. in Pagis (ref. [132]), but they are simply a description of potential future climates, without any thermal calculations.

9. Conclusions

A general conclusion from this work is that thermal calculations constitute the “easy” part of the much more general problem of the hydro-thermo-mechanical behaviour of a geological host rock under the influence of a heat-producing repository.

We have examined contributions from various countries, whose repository concepts are quite similar in principle, but different in their details: containers may be stacked in boreholes, lined up horizontally in drifts, or buried in a buffer material in rooms. This does not greatly modify the general modelling approach.

It is clear that at their present stage of development, models are not able to simultaneously cover all the scales, from the regional to the near-field: choices must be made as to what scale is appropriate for a particular aspect. Generally, a very detailed model must be restricted to a local region, which is either a sub-domain of a more general model, with boundary conditions extracted from this regional model, or bounded on the basis of symmetry considerations. In any case, the vertical extent of this local model must be sufficient to include realistic boundary conditions. In a regional model, it is possible to use a simplified representation of the source without loss of accuracy. The development of specific models for various scales, although cumbersome, may have advantages, because one is forced to correctly assess the orders of magnitude of various mechanisms to make the appropriate approximations.

The Equivalent Continuous Medium approach is well suited to the modelling of heat transfer, because this phenomenon is rather insensitive to the presence of fractures. Fractures must, however, be taken into account when the effect of heat on water trajectories is assessed. Generally, the density coupling for sparsely-fractured rocks is a one-way coupling: heat transfer is insensitive to the flow in fractures, but the flow in fractures can be modified by the temperature long after the thermal perturbation of the medium has vanished.

Various numerical techniques are available to solve the heat transfer equation: Finite Elements, Finite Differences, Distinct Elements or even analytical techniques.

These techniques have different abilities to deal with coupled mechanisms, but perform equally well for the heat diffusion equation. Thus, the results do not seem to depend greatly on the modelling techniques, because the heat conduction equation is rather robust and not prone to unstable solutions.

There seems to be little uncertainty regarding the value of thermal parameters (thermal conductivity and specific heat of the various materials), and as a consequence, little uncertainty regarding the results of thermal calculations in terms of temperature. This is especially true for saturated media. The major source of uncertainty in the predictions seems to be the behaviour of the bentonite, with respect to its water content : the saturation of the bentonite strongly affects its thermal conductivity, and furthermore, if the bentonite is only partly saturated, two-phase transport of water and heat can occur, making the modelling and predictions much more complex. More precisely, the variation in water content is difficult to predict with accuracy, which impacts on the thermal calculations. The possible existence of a scale effect has been proposed to explain discrepancies between field measurements and predictions based on parameters measured in the laboratory. However, this scale effect has, so far, not been demonstrated for thermal parameters, as is the case e.g., for the hydraulic conductivity.

The most elaborate modelling work found during this review seems to have taken place in Sweden: the concepts used in the various modelling exercises examined here are consistent, except for minor differences in parameters, and reflect the increasing power of numerical tools.

A large body of experimental evidence has been and still is being developed around the hydro-thermo-mechanical aspects. These experiments cover a variety of spatial and temporal scales. The modelling results obtained in connection with these experiments are generally in good agreement with the observations as far as temperature is concerned. At present, the most elaborate work (excluding the US programmes which concern a different hydrological situation) seems to be the FEBEX experiment, on the behaviour of the bentonite buffer.

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