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Guidance document on THM coupled processes in performance assessment (Benchpar)

Ove Stephansson (Coordinator)

GeoForschungsZentrum (GFZ), Germany

The Royal Institute of Technology (KTH), Sweden

John A. Hudson

Imperial College, London and Rock Engineering Consultants, United Kingdom

Johan Andersson

Streamflow AB, Sweden

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Summary

The objective of this Guidance Document is to provide advice on how to incorporate thermo-hydro-mechanical (THM) coupled processes into Performance Assessments (PAs) and design studies for radioactive waste disposal in geological formations to be experienced in a European context. The document has been generated by the EU research project BENCHPAR: Benchmark Tests and Guidance on Coupled Processes for Performance Assessment of Nuclear Waste Repositories.

The document starts in Section 1 with an explanation of why numerical analyses incorporating THM mechanisms are required for radioactive waste studies and provides background material on the subject. Then, the THM processes and their interactions are explained in Section 2. Three case examples of THM numerical analysis are presented in Section 3 to illustrate the type of work that can be conducted to study the near-field, upscaling, and the far-field. The importance and priority of the THM couplings are summarized in Section 4. Recommended soft and hard auditing procedures are presented in Section 5.

In this Guidance Document, we emphasize especially that the most important step in numerical modelling is not executing the calculations *per se*, but the earlier conceptualization of the problem regarding the dominant processes, the material properties and parameters, the engineering perturbations, and their mathematical presentations. The associated modelling component of addressing the uncertainties and estimating their influence on the results is similarly important. In other words, the specific models and codes should be studied first to evaluate the harmony between the nature of the problem and the nature of the codes. The practical use of particular numerical techniques will then be based on a sound strategic foundation. An associated listing of bullet point recommendations and issues for future directions for this THM subject area is given in Section 6.

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1. Introduction

1.1 Why numerical analyses are required for P/SA and repository design

Being able to model the behaviour of rock masses is of crucial interest for many applications. For radioactive waste repositories there are two related objectives associated with such modelling.

- Modelling the future evolution of a site with emphasis on how this evolution affects the safety functions (generally isolation and retention) is a key component of repository performance and safety assessments. Since the evolution needs to be assessed over time spans much longer than any attainable experiment, statements on evolution must be based on predictive numerical modelling. However, this does not mean that the models need to predict exactly what will happen in the future; the modelling needs to capture mechanisms and changes essential for understanding performance.
- Modelling the rock mass is also important for repository engineering, i.e. in deciding on repository design and in the related optimisation of the engineering works. However, in contrast to performance assessment applications, the rock mass response due to the engineering will be largely known once the underground facilities are constructed. The need for predictive modelling in this context is thus more related to optimising between what can be modelled prior to excavation and the consequences of adverse events during the excavation work.

There are two main challenges in predicting the behaviour of the rock mass: its evolution and response to disturbances are controlled by coupled, thermal, hydraulic, mechanical and chemical processes; and the properties of the rock vary in space in a complex and not fully predictable or quantifiable manner. A complete understanding, characterisation and modelling of the geosphere is unattainable; however, complete coverage of all the geometrical details and mechanical processes is never needed in practice. How comprehensively the coupled mechanisms have to be modelled should be related to the objectives of the modelling. This means that the allowable approximation may differ between P/SA and engineering applications — even if the modelling concerns the same rock mass.

1.1.1. What is Performance and Safety Assessment?

The objective of a safety assessment (SA) of a deep geological repository for nuclear waste is to produce a decision instrument based on a careful evaluation of factors affecting its performance. Such decisions may, for example, concern the need for further studies of a proposed site or concept, the selection of other sites for further characterisation, or ultimately the decision whether the repository at a specific site is (or will be) sufficiently safe to warrant a licence for construction, operation or sealing.

The OECD Nuclear Energy Agency has explored 10 recently conducted Safety or Performance Assessments (OCED/NEA, 1997). The study suggests that a “Safety Case” for the long term performance of a nuclear waste repository consists of:

- “A quantitative analysis of a set of processes that have been identified as most relevant to the overall performance of the disposal system and calculations of a measure of overall performance relevant to the given national regulatory regime, e.g. individual dose to members of a critical group, integrated total release of contaminants.”

- “Testing of arguments that a sufficient subset of processes has been analysed, appropriate models and data used, plus comparison of calculated measures of overall performance to regulatory limits and targets.”
- “A full trace of arguments and evidence that a sufficient set of processes has been analysed and appropriate models and data used; relevant overall measures of performance and safety are within acceptable ranges allowing for uncertainties. More qualitative, parallel lines of evidence and reasoning may be used to support results of the quantitative modelling and to indicate the overall safety of the system...”.

According to the OECD/NEA study, the first two of these steps are the safety assessment, and if the analysis is confined to a part of the repository system it is instead called "Performance Assessment". However, it should be recognised that different organisations use these words with slightly different meanings.

In general, it should be understood that a safety assessment and a safety case need not be a complete description of all processes and interactions that take place or will take place in a repository system. Only conditions that have, or could potentially be suspected to have, implications on safety need to be described. Detailed predictions of the evolution of the system are not needed if it can be shown that the evolution and its consequences are insignificant for safety considerations. Simplified models and assumptions could be made provided they can be shown to be 'conservative'. Furthermore, the arguments and the modelling do not necessarily need to be quantitative — bounding evaluations may be sufficient, even if it is still necessary to demonstrate enough physical understanding of the processes that affect the repository environment and evolution, such that the bounding assumptions could be justified.

1.1.2. Differences between Safety Assessment and engineering predictions

Designing and managing underground constructions require predictions of rock conditions and responses during construction. Rock construction implies significant disturbances to the rock, which means that coupled THM effects probably are more pronounced during construction than afterwards during the relatively uneventful post-closure phase. Having said this, it needs also to be understood that the requirements on engineering predictions are not the same as those made for safety assessment.

Engineering predictions are made as support for making decisions on design and (later on) construction. While such decisions may have far reaching practical and economical implications, they do not concern radiological hazards. Many engineering decisions do not concern issues of long term safety. Furthermore, the adequacy of predictions will be checked against the construction reality. Erroneous predictions may lead to poor engineering decisions, but not to radiological risk. This leads to less strict demands on engineering predictions compared to Safety Assessment, but engineering predictions are not unimportant.

Poor engineering decisions may jeopardise the repository project — no one would be interested in making underground excavations later found to be unsuitable for a repository. Furthermore, even if some engineering predictions concern issues of little relevance for long term safety, the ability to make these predictions would clearly enhance the confidence in the overall ability to make predictions (including those directly related to long term safety).

Consequently, in assessing the relevance of a THM coupling, it is important to consider whether its impact concerns engineering issues or safety issues. The latter should acquire special focus, but the former are still important.

1.1.3. Judging the relevance of THM-coupling

When considering the THM mechanisms, it is important to judge whether a given process has relevance to the repository performance, or if increasing the complexity of characterisation and modelling is actually required. The modelling has to be developed to a useable practical scheme, which captures the essence of the required processes. Some THM couplings will be concept, site, and waste-type specific, e.g. whether high-, medium- or low-level waste is being considered

Clearly, it needs to be understood that Safety Assessment concerns an evaluation whether a given repository concept in a (more or less defined) siting environment is safe in relation to pre-set safety criteria. Safety Assessment is not a means to describe and predict every aspect of the future evolution of the repository. Furthermore, criteria, concepts and siting environments change. This means that what is important in one concept may be totally irrelevant in others.

When evaluating the confidence in THM-predictions it is necessary to match the level of confidence with an understanding of 'how much confidence is needed'. There are three issues:

- the accuracy and precision of the THM prediction,
- the relative inaccuracy (uncertainty) in the THM prediction given the inherent spatial/temporal variability of the domain properties (i.e. geosphere/vault/engineered barrier system), and
- the relative importance of uncertainty in the predicted THM process/mechanism compared to others occurring in the vault/geosphere.

With regard to the first point, there needs to be a performance measure against which THM predictability can be judged and a means should be developed for quantifying the error made by neglecting/simplifying the coupling. Comparison against such measures is essential in order to make reasoned statements on predictability, stating reasonable expectations for THM predictions and evaluating the relative importance of THM processes/mechanisms for repository safety. In formulating the different BENCHPAR Work Packages, this need was foreseen and performance measures for each of the tasks were defined. In evaluating the outcome of the Work Packages, these measures have been assessed as well.

The second point related to the fact that the geosphere is heterogeneous and complete characterisation is problematic — so, given this, how accurate can our predictions be? If performance measures suggest a divergence between observed and predicted results is this a fundamental problem in understanding and accounting for important THM processes/mechanisms or is it simply an inability to completely characterise the domain and boundary conditions?

Lastly, the results should be placed into context with other PA issues relevant to repository safety. It may be in the end that THM process/mechanisms are relatively minor (i.e. compared to uncertainty in geosphere transport, canister failure rates, retardation factors, long-term climate change, parameter up-scaling, etc.). These aspects also have to be assessed and discussed.

1.2 Background on the mechanisms that need including in THM analyses

When we are modelling the behaviour of a rock mass for SA and engineering design purposes, and it is considered that there are significant thermo-hydro-mechanical-chemical interactions, the six main aspects of the modelling problem are as follows.

- Geological: site geometry, lithology, fractures
- Thermal: heat loads, heat flow
- Hydrological: water pressures, water flow
- Mechanical: rock stress, stiffness, strength
- Chemical: water chemistry, swelling rocks
- Engineering: effects of excavation

In a THMC model, the geology is taken into account via the host rock geometry and properties. For engineering, excavation perturbations are applied to the model and the main consequence is the Excavation Disturbed Zone. The construction of an underground excavation will lead to changes in the rocks surrounding the excavation, resulting in localized mechanical deformation, alteration in the stress distribution and changes in the water flow and hydraulic properties of the surrounding rock volume. This zone of altered properties is termed the Excavation Disturbed Zone (EDZ). Thus, all six GTHMCE aspects should be taken into account in a THMC model.

If we consider that there are individual binary interactions between these six aspects, there are $(6 \times 6 - 6) = 30$ separate interactions. The concept of such interactions and the use of an interaction matrix within rock engineering systems to conceptually identify these have been discussed by Hudson (1992). Note that the binary interactions define the individual linkages between the subjects; ternary and higher level interactions are considered as pathways through the binary interaction matrix (i.e. as concatenations of binary interactions). The structuring of the features, events and processes (FEPs) related to radioactive waste disposal within an interaction matrix has been used by SKB in Sweden (SKB, 1999).

However, it is not necessary to develop an all-encompassing model: it is only necessary to include those interactions that will significantly affect the predictive capability. Whether a particular interaction is required to be represented in the computer model depends on the significance of the interaction, given the objective of the modelling.

1.3 Background on numerical methods available and the THM mechanisms

A review of techniques, advances and outstanding issues in numerical modelling for rock mechanics and rock engineering has recently been written by Jing (2003). This paper is recommended for a detailed description of the numerical methods currently available. Two text passages in the conclusions of that paper are especially important in the current context.

- “The most important step in numerical modelling is not running the calculations, but the earlier ‘conceptualization’ of the problem regarding the dominant processes, properties, parameters and perturbations, and their mathematical presentations. The associated modelling component of addressing the uncertainties and estimating their relations to the results is

similarly important. The operator should not ‘dive in’ and just use specific approaches, codes and numerical models, but first consider the specific codes and models to evaluate the harmony between the nature of the problem and the nature of the codes, plus studying the main uncertainties and their potential effects on the results.”

- “Success in numerical modelling for rock mechanics and rock engineering depends almost entirely on the quality of the characterization of the fracture system geometry, physical behaviour of the individual fractures and the interaction between intersecting fractures....Today’s numerical modelling capability can handle very large scale and complex equations systems, but the quantitative representation of the physics of fractured rocks remains generally unsatisfactory, although much progress has been made in this direction.”

In fact, the full development of T-H-M-C modelling is still at an early stage. For example, we do not have satisfactory answers to the following questions. Do current codes provide the information that is required? How can the codes be validated? How can the codes or the approaches in applying them, be modified to fit the ambition of the modelling? What kind of quality control instruments need to be introduced? The BENCHPAR work has addressed some of these issues.

1.4 Purpose and content of this Guidance Document.

The objective of this Guidance Document is to provide advice on how to incorporate THM coupled processes into Performance Assessments (PAs) and design studies for radioactive waste disposal in geological formations to be experienced in a European context. The Guidance Document includes the background already described on why numerical analyses are required for performance assessment and repository design and the mechanisms that need including in such analyses.

The thermal, hydrological and mechanical (THM) processes and their interactions and couplings are described next in Section 2. An interaction matrix is also presented to illustrate how THM mechanisms, plus their interactions with geology and hydrogeochemistry, can be conceptually identified

Three modelling cases (the Benchmark tests in Work Packages 2-4 in the BENCHPAR project) are then described in Section 3 to illustrate the importance of THM couplings in the near-field, for upscaling from the near-field to the far-field, and in the far-field, respectively. An overview of each case example is presented together with the main findings of the numerical simulations. The relevance to the safety case and the performance measures are stated. The importance of couplings and the ratings of the importance are presented for each of the case examples. Finally the major uncertainties in modelling and parameter inputs are listed for the case examples.

The importance and the priority of the THM interactions is summarized in Section 4.

There is a need for technical auditing of the THM numerical analysis and this is described in Section 5. Here the term ‘technical auditing’ means examining the technical content of a THM numerical analysis to establish if it is adequate for the purpose. ‘Soft’ and ‘hard’ auditing procedures have been developed. A ‘soft audit’ enables the features of the modelling to be established and statements to be made concerning whether the right approach has been adopted in principle. A ‘hard audit’ involves detailed analysis of the modelling to establish the relevant variables, mechanisms and parameters, whether the modelling is relevant, and whether the design is appropriate and robust.

Finally, in Section 6, the Guidance Document includes recommendations for THM analyses and the likely future directions. The final results of the BENCHPAR project will be published as a series of reports by the Swedish Nuclear Power Inspectorate.

2 The THM Mechanisms

Considerations of deep geological radioactive waste disposal involves studies involving the coupling of thermal (T), hydrological (H), mechanical (M) and chemical (C) processes, although in the BENCHPAR project and this document the chemical processes have been omitted. The majority of repositories consist of the four system parts: waste/spent fuel, canister, buffer and backfill, and the geosphere. The studied THM mechanisms and processes in the BENCHPAR project were restricted to the buffer and backfill and the geosphere system.

2.1 Thermal processes

By heat transport from the waste or spent fuel via the canister and the buffer, the surrounding rock mass will be affected by primarily heat conduction and heat conductivity; heat capacity of the rock and its mineral constituents determines the process and the final temperature distribution. To a small extent, heat can be transported by convection of the groundwater, but this can normally be neglected for a waste repository. For stationary time independent conditions, the heat transport is governed by heat conductivity of the rock and its discontinuities. During transient conditions, like the situation in a waste repository, the rock ability to store heat will also play a role and this capacity is determined by the heat capacity and density of the rock. In general, the heat distribution in a repository can be described as a diffusion process governed by the diffusivity of the rock mass and its discontinuities.

In the Earth's crust there is a steady state heat transport from the warmer deep parts to the surface where cooling takes place due to heat transfer to the atmosphere and by radiation. The geothermal heat flow is essentially constant and is determined by the heat conduction of the rock and the geothermal gradient. The heat from the repository will be superimposed on the existing geothermal temperature.

The heat production from the radioactive waste and spent fuel will generate a heat wave that will transfer in all directions out from the repository. The process is transient and is determined by the total energy stored in the repository, the distribution geometry of the waste and the diffusivity of the rock mass. The heat distribution in the repository diminishes with time and reaches the peak temperature in the repository after ca. 100 years when the total effect has been reduced to about 70 percent. For a repository located at about 500 m depth, the heat wave will reach the surface after a couple of hundreds years. This means that the maximum temperature in the repository is independent of the conditions at the ground surface.

The geometry of the repository has a large influence on the temperature distribution. For a typical KBS-3 concept with vertical deposition of canisters in boreholes/shafts in the floor of a tunnel system, the effect density is about 7 W per square meter for a tunnel distance of 40 m and a distance of 6 m between the canisters. For a given canister effect and deposition geometry, the heat transport in the rock mass determines the temperature at the wall of the deposition hole, the buffer and canister. Therefore, the heat conductivity, heat capacity and density of the rock mass are the governing parameters, of which the conductivity is the most important. The proportions of different rock types and their stochastic distribution determine the effective heat conductivity

of the repository. Heat conductivity is known to vary with mineral content and temperature and less with pressure. Water filled fractures have a small influence on the temperature distribution.

Heat is transferred from the surface of the canister to the buffer, through the buffer and finally from the buffer directly to the surrounding rock mass or via the backfill in the tunnel system. At the initial phase of deposition, conduction via small open joints and fissures can take place. When the buffer is water saturated and the swelling is completed, heat transport takes place with conduction. Density, degree of water saturation and mineral composition determine the heat capacity of the bentonite buffer.

2.2 Hydraulic processes

The driving force for the groundwater flow in the geosphere is the differences in potential energy between two or several points in the geosphere system. The water pressure, water density and the vertical distance between the points determine the potential energy and the water density depends on the temperature and salinity. The amount of flow is determined by the size of the driving force and the permeability of the geosphere. For crystalline rocks, the flow properties are governed by the structure and stress field of the fractured rock mass and the transmissivity of the individual fractures. The water temperature and chemistry determine the viscosity and flow properties of the water. The groundwater flow is of central importance in the safety analysis of a repository. The flow will influence the chemical environment of the repository and is of utmost importance for transport of radionuclides from the repository to the biosphere.

The most common approach for determination of groundwater flow in the geosphere is based on Darcy's law — where the flow per surface area is proportional to the gradient multiplied by the flow property (permeability) of the medium. The flow vector consists of the sum of the pressure gradient and the gradient governed by the gravity forces, and the flow system is governed by the interaction between recharge and discharge areas. The flow length and flow paths of the water particles are determined by the topography, water density and the water flow properties of the rock and soil masses.

Close to sea shorelines, saline groundwater appears and the salinity typically increases with depth. An increasing salt content will increase the water density and decrease the groundwater flow, and at great depth lead to stagnant conditions. Heat conduction from the waste will also cause heat of the groundwater around a repository and the density contrast between cold and warm water might cause convection currents.

Results of hydraulic field tests have shown that individual and groups of fractures and fracture zones have large variation in hydraulic properties. The transmissivity of single fractures is roughly proportional to the third power of the fracture aperture. This means that the transmissivity can vary several tens of orders of magnitude in the same rock type.

Glaciation of the Earth's crust causes a depression of the crust from the weight of the ice and a new equilibrium between the crust and mantle. Melting of the ice causes disequilibria and the crust will rebound and thereby the topography and groundwater flow will change at coastal areas. Future climate changes will also cause the growth of new glaciers and related permafrost, which leads to changes in the hydraulic conditions at a repository site.

The water transport in the buffer at unsaturated conditions is a complex process which depends on temperature, water content in different parts of the buffer and the content of smectite in the

buffer material. The most important driving force for reaching water saturation and swelling of the bentonite is the suction in the pores of the buffer which draws the water from the surrounding rock mass. Therefore, it is of utmost importance that there exists enough water in the rock mass to provide for the suction and swelling. The following hydraulic processes are of importance. The transport of water is driven by the pressure gradient in the water and the osmotic gradient and the transport of water in vapour phase by the pressure gradient in the water, the temperature gradient and the osmotic gradient. In addition, the phase changes between water and steam causes precipitation and condensation. Finally, the thermal expansion and compression of water and air will affect the hydraulic conditions in the buffer and backfill. The majority of these processes have been studied in the BENCHPAR project and results from a case example are presented in Section 3.1.

One of the key questions regarding the function of the high compacted bentonite is its ability to saturate, which is a function of the total water inflow to the deposition hole and the distribution of water at the surface of the bentonite. Few water bearing fractures in combination with a low permeable matrix might cause uneven swelling and jeopardize the function of the buffer. Drilling of the deposition hole causes an excavation disturbed zone (EDZ) at the wall of the borehole and this zone facilitates an even distribution of the water. The swelling ability is reduced and the permeability increases for bentonite emplacement in contact with saline groundwater.

2.3 Mechanical processes

The rock mass of the Earth's crust has the ability to provide the mechanical and stability integrity of a waste repository over short and very long time-spans. The rock should protect the engineered barriers system and prevent any damage to the waste canisters.

There are basically three mechanical processes and states that need to be explored and understood for the design, construction, operation and closure of a repository: namely rock deformability, rock strength and rock stresses. The rock mass consists of intact rock and discontinuities, the latter being natural fractures in the mechanical continuum, such as joints and fractures. When the rock mass is loaded, the intact rock or matrix deforms in a way that can be described by simple stress-deformation relations when the load is small to moderate. The joints and fractures can deform by compression, shear and dilatancy.

The rock mass response to the loading is a superposition of the deformation of the intact rock and the discontinuities. Frequency, orientation and mechanical properties of the discontinuities play a major role for the rock mass deformability. In addition, the deformability of rocks is scale-dependent and large rock masses are less stiff, i.e. more compliant. The stresses generated in a rock mass due to deformation in compression, tension and shear can be described with relatively simple stress-strain relations. For small deformations, the process is elastic and hence reversible and can be described by the theory of elasticity and the associated elastic parameters Young's modulus and Poisson's ratio, for an isotropic rock. Similarly, the deformation of discontinuities can be characterized by the normal and shear stiffnesses (and the associated cross-stiffnesses) which relate the stress and displacement normal to and along the plane of the discontinuity, respectively. From the known deformability of the intact rock and the stiffness of the discontinuities, the rock mass deformability can be estimated theoretically, numerically or empirically.

For large deformations of intact rock, discontinuities and rock masses, the deformability is no longer reversible and non-reversible, inelastic deformation will be manifested. For additional loading and deformation, fracturing of the intact rock and/or shearing takes place along the discontinuities and the strength of the rock mass and its components are reached. The strength of a rock mechanics system is determined by the loading conditions and the strength of the intact rock, discontinuities or the rock mass. Existing failure criteria for rock materials describe the relation between the three principal stresses or between the shear stress and the normal stress acting on a defined surface in the rock system. The Mohr-Coulomb failure criterion and the Hoek-Brown failure criterion are the two most common criteria used in rock mechanics. The former can be applied to intact rock, discontinuities and the rock mass, and the Hoek-Brown criterion to intact rock and rock masses. Both criteria are applied for two-dimensional analyses where the influence of the intermediate principal stress is omitted.

The pre-existing rock stress and how it is affected by engineering activities is the third mechanical state or parameter to consider for THM coupling. The virgin state of stress at a site is governed by the gravitational stress from the weight of the overburden and by the tectonic stresses. The gravitational stress increases more or less linearly with depth, depending on the rock density, so the vertical depth below ground surface governs the magnitude of the vertical stress component. The confinement at depth generates a related horizontal gravitational stress component that is superimposed on the horizontal tectonic stress resulting from active plate movements in the Earth's crust. The orientation of the horizontal stress component over large areas is determined by the direction of the plate movements.

Major fault and shear zones in the crust cause natural perturbations of the stress field, the reorientation of the stresses being determined by the strength and deformability of the discontinuity. The stress field at a potential repository site has to be measured in boreholes and/or from shafts and tunnels of a repository. The magnitude and orientation of the measured stresses are important parameters for the design and construction work and as boundary conditions for the modelling of the THM processes for safety and performance assessment.

The buffer and the rock mass in a repository mainly influence each other *thermally* by heat flow, *hydraulically* by groundwater flow, *mechanically* when the buffer absorbs water from the rock and swells, and also *chemically* by exchange of solutes between groundwater and pore water in the buffer. On absorbing water, the buffer and backfill swell and a swelling pressure is built up, acting in all directions, but importantly towards the wall of the deposition holes and the tunnel walls and floor. The swelling pressure of the buffer may reach about 10 MPa and can cause opening of existing discontinuities or fracturing at the wall of the deposition hole. The swelling and shrinking and the generated swelling pressure is a function of the bentonite density, smectite content, pore water composition and the degree of saturation. The influence of some of these variables and the THM couplings has been studied in the BENCHPAR project for a KBS-3 system, see Section 3.1.

A mechanically stable, although sometimes limiting equilibrium, state exists initially in the geosphere, which is determined by the virgin rock stresses and the strength of the rock mass and the large-scale fractures, plus the changes to which the construction of the repository has given rise. The mechanical evolution and state of stability is determined by how the geosphere responds to the different mechanical loads to which it is subjected. Loads may consist of the thermal expansion to which the heating of the repository leads, the pressure from swelling buffer/backfill, effects of earthquakes, and the large-scale tectonic evolution over geologic times.

Changes in the geosphere due to glaciation, permafrost, deglaciation, glacial rebound, neotectonics, etc., may cause new fracturing and/or reactivation of existing fractures and fracture zones. Movements of intact rocks may also occur. Some of these processes have been studied in one of the bench-mark tests of the BENCHPAR project, see Section 3.3.

2.4 Interactions between the THM processes and coupling the processes

In the numerical modelling, we not only have to consider the T, H and M components in isolation but also to consider their interactions. There are two aspects to this:

- identifying the interactions; and

- having the appropriate algorithms in the modelling code.

A useful tool at the outset for conceptually identifying the interactions is to use an interaction matrix. This type of matrix with example interactions is shown in Fig. 2.1 for five disciplines (geology, rock mechanics, hydrogeology, hydrogeochemistry and thermal properties/processes). The main subjects are placed along the leading diagonal of the matrix from the top left to the bottom right. Note that there is a clockwise interaction convention in the matrix so that, for example, the influence of rock mechanics processes on hydrogeology processes are located in Box 2,3, whereas the influences of hydrogeology processes on rock mechanics processes are located in Box 3,2.

The generation of this type of interaction matrix is useful for establishing the nature of the interactions relevant to a particular THM problem and prior to deciding which interactions require to be reflected in the numerical code. It will not be possible to include them all, but a further assessment of the significance of this can be developed by using the technical auditing procedures described in Section 5.

The basic principle of an interaction matrix is to list the parameters defining the properties and conditions in the physical components of the system studied along the leading diagonal elements of a square matrix, see Fig 2.1. Interactive events and processes that are influenced by and affect the properties and conditions defined in the leading diagonal elements of the matrix occur in the off-diagonal elements of the matrix. The development of an interaction matrix consists of the following steps:

- Selecting the state variables

- Identifying the off-diagonal interactions

- Ranking the importance of the interactions

- All steps and decisions should be documented.

1,1 Geology	1,2 Rock inhomogeneity and anisotropy, & fractures (geometry, etc.) affects rock properties/stresses	1,3 Rock porosity, rock mass permeability, and water-rock interaction affects water flow	1,4 Rock mineralogical composition and geometry of fractures affects hydrogeochemistry	1,5 Mineralogical composition, porosity, textural and structural anisotropy effects
2,1 Stress data affecting the geo-interpretation of fracture systems and rock mass	2,2 Rock Mechanics	2,3 Spatial distribution of in situ stress and EDZ influences the hydrogeological regime	2,4 Stress changes near fractures zones affecting flow may change precipitation	2,5 Rocks & fracture zones subjected to higher stresses may be more thermally conductive
3,1 Hydrogeological tests and measures can affect the geo-interpretation of permeable features	3,2 Water pressure changes the effective stress	3,3 Hydro-Geology	3,4 The flow pattern affects dilution and mixing	3,5 The flow pattern will affect the temperature due to convection effects
4,1 Hydrogeochemistry interpretation affecting the interpretation of fracture min.rel.	4,2 Precipitation in fractures affects the fracture stiffnesses, strengths and creep properties	4,3 Effects of ground-water age, density, viscosity, and dissolution and precipitation	4,4 Hydro-geo-chemistry	4,5 No interaction
5,1 Thermal anisotropy and measurement affecting the geo-interpretation	5,2 Change in temperature can change the local stress, possibly leading to failure	5,3 Temperature gradients and thermal expansion in rock/fractures affect the water flow	5,4 Dissolution and precipitation enhanced by thermal gradients	5,5 Thermal Properties

Fig 2.1. Interaction matrix illustrating the interactions between the mechanisms associated with the different disciplines of geology, rock mechanics, hydrogeology, hydrogeochemistry and thermal properties/processes.

Thus, the first step is to select parameters required to describe the properties and conditions in the physical components of the system and to list them as the leading diagonal elements of the matrix. This is done by exploring how the system state can be described in terms of physical components, spatial and temporal extensions of the system, and initial and boundary conditions of the system.

The second step is to identify the binary interactions between the diagonal elements by going through all the off-diagonal elements in the matrices and using a clock-wise convention for the direction of the interactions. All interactions should be binary, i.e. they should be direct interactions between the variables in two leading diagonal boxes and not be a path via a variable in a third diagonal box. The identification process should be developed systematically with all the off-diagonal elements. A short description of the interaction should be documented, together with the variables in the two leading diagonal elements that are involved in the interaction.

Even if there are no interactions in an off-diagonal box, this should also be documented and if possible the reason for not finding any interacting event or process. For example, if the physical components defined by the variables in two diagonal elements are physically isolated, there will be no direct dependence between the variables in these diagonal elements. This does not preclude the possibility that the variables may be indirectly dependent via a path involving additional diagonal elements, but this will be established from subsequent analysis of mechanism pathways through the interaction matrix of binary interactions.

The last step, see Section 4.1 for further explanation, is to judge the importance of the interactions using a pre-defined priority scale for the problem in hand. The question should be asked whether the interaction is crucial, relevant or only marginally important for assessing the relevant performance of the system. A simple colour coding (e.g. red, yellow, green) can be used for displaying this. The prioritisation could thus be an effective means of reducing and visualizing the complexity of the system description — such that it focuses on the important aspects of the problem. However, one should note that the prioritisation is problem dependent, i.e. the importance of the rankings is made in relation to the problem being analysed and is also subjective. Experience is needed to make appropriate priorities. For example, the ingress of water to the near surface parts of an access tunnel may be much less important than the ingress of water deeper down in the repository.

3 Case Examples of THM Numerical Analyses

3.1 Case example 1: Safety issues related to near-field THM processes

3.1.1 Overview

The near-field work (Work Package 2 of BENCHPAR) was aimed at scoping calculations in order to determine how T-H-M processes can influence the flow field, as well as the structural integrity of the geological and engineered barriers in the near-field of a typical repository. The problem was further divided into three sub-tasks: WP2A – the calibration analysis of coupled THM models and computer codes against the Kamaishi in situ THM experiments (Jing, ed., 2001); WP2B – the simulation of the generic near-field repository behaviour without discrete fractures (Nguyen and Jing eds., 2003); and WP2C – the simulation of the generic near-field repository behaviour with discrete fractures. Scoping calculations of different combinations of coupling mechanisms were performed for WP2B and WP2C to examine their relative importance in the context of the performance of the near-field repository.

3.1.2 Main findings

As a result of the additional calibration measures, the results from the simplified axisymmetric model used in the re-evaluation of the Kamaishi mine experiment (WP2-A) showed general improvement over the original models used in the prediction phase, especially in the following aspects:

- Calculated values of temperature agree very well with the experimental values, for all teams.
- Generally improved stress and strain behaviour in the bentonite, at least qualitatively though, with the measured results.
- The water content near the heater (at point 1) is relatively well predicted by all teams, although the saturation front at the bentonite/rock interface are still predicted to advance much faster than in reality.

In general, the mechanical behaviour of the buffer is complex, with forces contributing from shrinking/swelling in all part of the bentonite, external stress from the thermal expansion of the heater and rock, and internal thermal expansion of the bentonite itself. However, a reasonable prediction of the mechanical behaviour can be achieved if all relevant bentonite properties are known from laboratory tests.

For the typical repository considered in WP2-B, only the full THM analysis predicts some localized rock mass failure around the boreholes, which might in turn result in a zone of higher permeability. Other important effects of the THM and HM coupling would be on the stress developed in the buffer, which would transfer to the canister and influence its stability. From a safety point of view, engineering measures could be easily be carried out to minimize these coupled effects. From the results of the present work, it appears that from a technical point of view the effect of coupling will be either short lived (several decades to 100 years) and hence would not impact on long term (thousands to hundred of thousand years) safety issues, or could be rectified by adequate design and operational methodology (e.g. avoid over-cooling the galleries).

3.1.3 Relevance to the safety case?

From a safety point of view, engineering measures could be easily carried out to minimize the coupled effects. From the results of the present work, it appears that, from a technical point of view, and as mentioned, the effect of coupling will be either short-lived (several decades to 100 years) and would not impact on long term (thousands to hundred of thousand years) safety issues, or could be rectified by adequate design and operational methodology (e.g. avoid over-cooling the galleries).

3.1.4 Importance of couplings

Table 3.1 summarises the effect of different degrees of coupling on the key performance and safety indicators in the near field of a repository. The rating of low, medium and high is rather qualitative and arbitrary, as explained in the preceding discussion. The definitions of low, medium and high are qualitative and given in the text. This Table is also dependent on the case and scenario being analyzed and no generalization should be made.

Table 3.1 WP2: The effect of different degrees of coupling on the key performance and safety indicators in the near field as assessed in WP2 (Table 7.6 in Nguyen and Jing, eds., 2003)

	Temperature	Resaturation	Swelling stress	Rock mass stability	Rock mass permeability
THM	Low	Medium/High	High	High	Medium/high
TH	Low	Medium	-	-	Medium
TM	Low	-	Low	Low	Medium
HM		Low	High	Low	Low

3.1.5 Uncertainties

The influence of the host rock properties (e.g. permeability) on the long-term safety seems to be much more important than coupling, since one has much less control over these properties. However, for confidence building and demonstration purposes, a fully coupled approach is necessary to interpret monitoring data that would be collected the first few decades after repository closure, since coupled processes would prevail during that period of time.

3.2 Case Example 2: Upscaling from the near-field to the far-field

3.2.1 Overview

Work Package 3 of BENCHPAR concerned the upscaling THM processes in a fractured rock mass and its significance for large-scale repository performance assessment. For an overview see Andersson et al. (2003). The work is primarily concerned with the extent to which various thermo-hydro-mechanical couplings in a fractured rock mass adjacent to a repository are significant in terms of solute transport typically calculated in large-scale repository performance assessments. Since the presence of even quite small fractures may control the hydraulic, mechanical and coupled hydro-mechanical behaviour of the rock mass, a key aspect of the work has been to explore the extent to which these fractures can be upscaled and represented by 'equivalent' continuum properties in appropriate PA calculations.

From these general aims, the WP was set-up as a numerical study of a large scale reference problem. Analysing this reference problem should:

- help explore how different means of simplifying the geometrical detail of a site, with its implications for model parameters and 'upscaling' impacts on model predictions of relevance to repository performance;
- explore to what extent the THM-coupling needs to be considered in relation to PA-measures; and
- compare the uncertainties in upscaling (both in relation to uncertainty on how to upscale and uncertainty that arises due to the upscaling processes) and in THM couplings with the inherent uncertainty and spatial variability of the site specific data.

Furthermore, it has been an essential component of the work that individual teams not only produce numerical results but are forced to make their own judgements and to provide the proper justification for their conclusions based on their analysis. It should also be understood that conclusions drawn will partly be specific to the problem analysed, in particular as it mainly concerns the 2D application. This means that specific conclusions may have limited applicability to real problems in 3D. Still, the methodology used and developed within the WP should be useful for analysing yet more complicated problems.

The reference problem concerns the far-field groundwater flow and transport for a situation where a heat producing repository is placed in a fractured rock medium. Radionuclides potentially released from the repository may migrate via the groundwater flow and thus reach the biosphere. Specific issues at stake are:

- how to assess the far-field hydraulic and transport properties when most data stem from small scale (borehole) tests,
- what is the impact of potential mechanical and hydraulic couplings, and
- if MH or HM couplings are significant, how would they affect the upscaling?

The relevant data, and boundary conditions, for the rock formations and fault are based on Sellafield data. The data are in the form of statistical distributions of properties. Typically, most

of the data concern measurements at the small scale, whereas, the problem to be studied mainly concerns the large scale.

The study concerns the impact on performance. The significance of different assumptions and methods should thus be compared through specified measures relevant to the performance being explored (far-field flow and migration). Furthermore, some intermediate measures, i.e. resulting upscaled parameter values, are worthwhile to compare.

3.2.2 Main findings

Several conclusions can be drawn from the individual team analyses, as well as from the interaction discussions held during Workshops and Task Force meetings. Interpretation of given data constitutes a major source of uncertainty. During the course of the project, it was certainly felt that these interpretation uncertainties could have a large impact on the overall modelling uncertainty. Differences between teams in estimating effective permeability appear to depend essentially on whether the team used given apertures as input — and then calculated fracture transmissivity using the cubic law — or if the hydraulic test data were used to calibrate the fracture transmissivity distribution. Furthermore, assumptions used as regards fracture size versus aperture (or permeability) are not really validated. Different assumptions for this would, although not really tested in the Task, lead to large differences in upscaled properties. The calculated effective rock mass deformation modulus differs between teams, but all teams include the ‘given’ value of the test case. It appears that this problem is relatively ‘well behaved’.

Despite the preliminary nature of the HM analysis conducted, some general remarks could be made. If modelling uses relaxed initial apertures as input, the HM coupling is essential for capturing realistic permeabilities at depth. However, this does not necessarily imply that the HM couplings need to be considered. The fact that the aperture versus stress relation reaches a threshold value indicates that the more normal practice of fitting hydraulic properties to results of hydraulic tests is warranted. A key process, where there still is uncertainty is the relation between hydraulic residual aperture and maximum mechanical aperture, R_b . Evidently this has a strong influence on the impact of the HM coupling. Related to this is the indication found on the significance of the increase of differential stress results in increasing the permeability (when applying the non-linear stiffness model for fractures) and in channelling of flow path (potentially caused by fracture dilation).

Despite the relatively limited amount of large scale analyses conducted within the Task, some general remarks seem possible. It is suggested that, because the stress is so high at the depth of the repository, fractures are almost completely compressed mechanically and the permeability is approaching its residual value. Therefore, further stress increase due to thermal stresses would not significantly reduce the permeability. Also the TH effects, due to buoyancy, are relatively limited and would add an uncertainty in the order of a factor of two or so.

These observations support the conclusion that it is the upscaling of hydraulic properties, rather than the added complication of T and M couplings, which are the main sources of uncertainty in a problem of this nature. The added disturbance, in relation to in situ stress, is small in the far-field of a deep repository. Yet, understanding the stress/permeability relation is important for understanding the nature of the permeability field.

It can also be noted that most conclusions to be drawn from the large scale analyses could already be drawn from studying the intermediate performance measures such as permeability, deformation modulus and permeability versus stress relations.

3.2.3 Relevance to safety case and performance measures

The scale of PA-models, or at least far-field radionuclide transport models, is usually large compared to the scale where there is some understanding and data on HM couplings. This raises several issues.

- How should coupled processes and associated parameters be upscaled?
- Are the HM couplings significant in relation to the geometrical factors controlling the upscaling of permeability and rock mass mechanical properties (such as deformation modulus)?
- Are couplings at all significant compared to other uncertainties (network geometry, hydraulic properties, fracture constitutive laws)?
- What are the site characterisation implications?

The Work Package was designed to address these issues.

Ultimately, the performance measure for a repository PA would be doses or risk; however, in order not to introduce too many assumptions about the waste, release mechanisms or the retention properties of different species, the general performance measures being studied here are restricted to the groundwater specific contribution to retention. The research teams were thus asked to predict the following.

- Flow related migration parameter in the form of ‘transit time distributions’ and ‘transport resistance distributions’ at two output surfaces.
- Intermediate results of upscaling (effective parameters) such as effective permeability and rock mass deformation modulus for different block sizes.

3.2.4 Importance of couplings

Table 3.2 shows the assessed importance of the different couplings. In short, it is not evident that there are any highly significant THM couplings to be considered for this problem. Upscaling permeability from small scale measurements is indeed a difficult task, but there is little evidence from the test case to suggest that the upscaling also needs to consider the added complexity of the THM-coupled effects.

Table 3.2 WP 3: Assessed Importance of Couplings

Coupling	Rating	Comments
TH	Low	Not significant at the large scale
TM	Low	
HT	Low	

HM	Potentially important	Considered potentially significant by most groups. Important starting point in DFN upscaling, but not (yet) proven to be necessary to consider given other uncertainties, remembering that hydraulic data are sampled at appropriate depths.
MT	Low	
MH	Potentially important	See HM

3.2.5 Uncertainties

It appears that the main uncertainties encountered in WP3 concern upscaling the parameters of individual processes. The currently listed major uncertainties include the following.

- Conceptualisation of fracture network data (the resulting upscaling is also very sensitive to this).
- Results sensitive to interpretation of fracture data.
- Software limitations, especially with hydromechanical codes

The findings certainly suggest that the THM uncertainties in this case are small in relation to the upscaling and geometrical uncertainties explored.

3.3 Case Example 3: Impact of glaciation and deglaciation on post-closure performance

Case Example 3 (WP4) is primarily concerned with the coupled hydro-mechanical (HM) impacts of one or more cycles of glaciation and deglaciation in the long-term (up to 100 000 years) and post-closure performance of the geosphere in which a repository is located (Boulton et al., 2003). A performance assessment of a deep repository consists of an analysis of the changes through time in the disposal facility as a consequence of both internal and external forces. Groups of coupled processes are linked together in a description of integrated evolution through time. The primary purpose of WP 4 was to develop modelling tools at a site scale for simulation of climate-driven boundary conditions (ice sheet loading, groundwater hydraulics and permafrost) and to illustrate the magnitude of some T-M-H impacts in the far field in the context of a PA.

The objectives of the WP were therefore:

- to study, by analytical and/or numerical modelling, the impact of a 100 ka glaciation-deglaciation cycle on the long-term evolution of a fractured rock mass in which a generic repository is located;
- to assess the impact of the glaciation/deglaciation cycle on the coupled thermo-hydro-mechanical responses of the far field system around a repository and on its long-term performance in waste isolation;
- to investigate/demonstrate the technical feasibility of deep geological disposal in hard rocks and improve the scientific basis for safety assessment and the strengthening of public confidence in safety assessment methodology.

The involved teams have focused on simulating glaciation in a way that can be tested by geological observations, and applied the model to suggest sub-surface impacts at specific sites to explore the implications for safety assessments. Simulations have been conducted for two sites, the Äspö site in Sweden and the Whiteshell site in Canada, designed to explore the impact of the growth and decay during the last glacial cycle of permafrost and ice sheet development.

The successive steps in the simulations are:

- Step 1 – Simulation of the climate drive, where the pattern of climate change is derived from the record from the Greenland ice sheet, adapted to the region using palaeo-climatic data from southern Canada and the northern USA and synoptic extrapolations.
- Step 2 – Ice sheet loading and basal thermal and hydrological regime using a thermo-mechanically coupled, transient ice sheet model (Boulton and Payne, 1994). The model is coupled with the Earth model of Lambeck et al. (1998) and driven by the climate function over a prescribed topography. The model computes the temperature at the base of the ice sheet and the rate of basal melting in time and space.
- Step 3 – Determination of permafrost distribution using a transient model of permafrost development (Mikkola & Hartikainen, 2001). The model is driven directly by the climate function when there is no ice sheet present and when the ice overrides the site, the temperature at the base of the ice sheet is used as a boundary condition for permafrost development.
- Step 4 – Simulation of groundwater flow, pressures and states of geosphere stress. The coupling between the permafrost and ice sheet are used to determine the transient response of the groundwater system and the state of rock stress along a 2D section parallel to ice flow. Investigation of groundwater flow and geosphere stresses and strains have also been undertaken for steady state and transient conditions along sections both parallel and transverse to ice flow using the ABAQUS and MOTIF codes.

3.3.1 Main findings

The climate function is used to drive a glaciological model of the Laurentide ice sheet through the last glacial cycle. It suggests that the Whiteshell site was glaciated at about 60 ka and during the glacial maximum, between about 22.5 ka and 11 ka, which is compatible with geological evidence from the region. The maximum ice sheet thickness at the site is modelled as 3000 m, which is likely to be an over-estimate. The model computes basal melt rates, and from a simplified, 1D description of hydraulic conductivity, computes the spacing of subglacial channels that would be required to drain the ice sheet bed.

The longitudinal head gradients associated with the ice front and the transverse gradients associated with channels are much greater than for the modern gradient. This means flow velocities one to two orders of magnitude faster than modern values and the generation of strong vertical flow components. Furthermore, the computed ground surface temperatures at the ice/bed interface, at 60 ka and between 22 ka and 11 ka, are higher than extra-glacial temperatures because of the insulating and heating effect of the ice sheet.

The temperature forcing function has been used to compute the evolution of permafrost thickness through the glacial cycle, together with unfrozen water content, the increase of salinity due to

freezing, and the magnitude of frost heave. Computed permafrost depths are of the same order as anticipated repository depths. Permafrost progressively decays beneath the glacier.

Strong groundwater flows, up to 2 orders of magnitude greater than in the non-glacial state, are generated beneath the glacier and beneath permafrost that extends beneath the glacier. Where permafrost is thin, significant water overpressures can develop and are enough to generate hydraulic jacking of bedrock.

The consequences of glaciation at greater depth are as follows.

- A rapid increase of head during the first 1000 years of glaciation.
- A rapid transmission of these heads through the fracture systems, producing much higher, early, transient heads than in the repository zone.
- During the glacier advance over the site, there is a large horizontal hydraulic gradient due to compression of pores by ice loading.
- As the area is completely covered by the ice sheet, a strong downwards hydraulic gradient develops, of as much as 3-5 m/m.
- At depth the excess water pressure is about 1/3 of the ice pressure.
- During ice sheet retreat, the gradient reverses, and is sustained, together with residual excess pressures of as much as 250 m at 800 m depth.
- Pressures in fracture zones decay rapidly after deglaciation.

The change in effective stress is relatively small as the increase in ice load is largely compensated by the increased groundwater head (however, there is a transient effect, as the former is instantaneous whilst the latter diffuses through the system). There is, therefore, very little rotation of principal effective stresses. Even in dead-end horizontal fractures, there is no generation of tensile stresses and therefore no hydraulic jacking at depth. No shear failure is predicted.

3.3.2 Relevance to safety case?

Boulton et al. (2003) conclude that safety assessments of the disposal of long lived radioactive wastes in the middle to high latitudes of the northern hemisphere must recognise that these areas have been repeatedly glaciated in the recent geological past, and that, were it not for the prospect of human induced global warming, we would expect an imminent descent into glaciation.

Glaciation has the potential to influence strongly the geosphere to the preferred depths for deep disposal sites of between 500 and 1000 m. The strongest potential impacts in periods of glaciation are associated with the extension of ice sheets and perennial ground freezing to create 'permafrost' to depths of several hundred metres. The involved processes are the product of a system driven by the Earth's climate and characterised by strong thermo-hydro-mechanical coupling, in which both chemical processes and transient phenomena are important.

Boulton et al. (2003) also conclude that although models of glacier-groundwater, glacier-permafrost-groundwater, glacier-groundwater-shallow failure systems have been presented, WP 4

is the first attempt to assess impacts at repository depths using site specific data. The results provide valuable insights into the magnitude and rate of change of site-specific hydrogeologic and geomechanical properties in response to external, transient climate forcing.

The most important general conclusions of BMT2 are that:

- glaciation occurs on a depth scale that is relevant to the safety of repositories buried several 100s of metres beneath the surface;
- glaciation occurs on timescales that are relevant to safety assessments for long lived waste; and
- assessed impacts implies transient, but several orders of magnitude, effects on groundwater flow.

The coupled processes connected to glaciation must be considered in safety assessments.

3.3.3 Importance of couplings

While the analysis points out several potentially important effects of future glaciations, only some THM couplings need to be considered. For the analyses of the Whiteshell site:

- the Hydro-Mechanical coupling effects on pore pressure are significant, as there are high residual pore pressures for 1000s of years after the glacier has retreated from the site,
- the Thermal impact on hydrology and mechanics may be significant in terms of permafrost, since permafrost may develop at repository depths,
- the Hydro-Mechanical impact in terms of potential hydraulic jacking at depth is not likely to be important,
- the impact on stress and mechanical stability at depth is minor.

Table 3.3 displays the assessed importance of the different couplings in Case Example 3. In addition, four separate components are used: namely, a climate model, an ice sheet-earth model, a permafrost model and an earth hydro-mechanical earth model. The ice sheet-permafrost models are weakly coupled, but the climate and hydro-mechanical earth models are uncoupled from other components. The development of a model in which the system is fully coupled and driven only by global climate, with feedbacks between the ice sheet and local climate is necessary if the full consequences of coupling are to be understood.

Table 3.3 Case Example 3: Assessed Importance of Couplings

Coupling	Rating	Comments
TH, HT	Low (High in terms of permafrost)	the thermal impact on hydrology and mechanics may be significant in terms of permafrost since permafrost may develop at repository depths;
TM, MT	Low (High in terms of	see above

permafrost)

HM, MH pore pressure	High	high residual pore pressure for 1000s of years after glacier has retreated from the site
HM, MH hydraulic jacking and stress	Low	the Hydro-Mechanical impact in terms of potential hydraulic jacking at depth is unlikely to be important; the impact on stress and mechanical stability at depth is minor;

3.3.4 Uncertainties

The following main uncertainties are related to Case Example 3.

- External climate driving ice sheet model.
- Site-specific properties (rock type, fracture network geometry & connectivity, hydraulic properties, fracture zone strength) and scaling.
- Boundary conditions, especially the hydraulic and mechanical state in the ice and in the bedrock at the ice/bedrock boundary, but also the hydraulic boundary conditions at the vertical boundaries.
- Model approximations, e.g. influence of salinity on flow omitted, representation of permafrost in HM models, mesh fineness, model size.

The importance of, e.g., spatial variability of rock mass permeability in relation to the process uncertainty is difficult to assess. The uncertainties due to THM coupling are not a subset of uncertainties due to spatial variability. It is judged that the two types of uncertainties are comparable in magnitude for the case example.

4 Importance and Priority of the THM Interactions

4.1 Identifying the mechanisms appropriate for a particular modelling exercise

In Section 2.4 on the THM mechanisms, an interaction matrix was presented to illustrate how one can initially identify the interactive THM mechanisms, plus their interaction with geology and hydrogeochemistry. This is the first step: to identify the mechanisms. The next step is to decide whether these mechanisms have ‘high’, ‘medium’, ‘low’ or ‘no’ significance. In the same way as for compiling the original interaction matrix through group discussion, so the interactions can be ranked by expert groups. The interactions in the example matrix presented earlier (Fig. 2.1) have been ranked in this way in Fig 4.1, i.e. not via the actual numerical modelling. It is emphasized that this is an example matrix; any group concerned with modelling should generate their own interaction matrix to ensure that all the features of their particular exercise have been taken into account.

Conclusions relating to the significance of the interactions and integration of the disciplines or the THM processes can then be drawn. Of the 20 interaction boxes in the example 5x5 interaction matrix in Figure 4.1, there is only one box in which no significant interaction was identified. Thus, there is a large degree of interaction in the system.

It is recommended that the following points be considered after completion of the interaction matrix.

Was the identification of the interactions straightforward? Is there a consistent inter-disciplinary understanding of the complete interactive model system?

Of the interaction boxes in the interaction matrix, are most boxes filled? Is there a large degree of interaction between the subjects on the leading diagonal?

Is there inter-disciplinary agreement about the significance ratings? If so, this indicates that the different disciplines have a consistent view of the significances of the different interactions.

1,1 Geology	1,2 (High) Rock inhomogeneity and anisotropy, & fractures (geometry, etc.) affects rock properties/stresses	1,3 (High) Rock porosity, rock mass permeability, and water-rock interaction affects water flow	1,4 (High) Rock mineralogical composition and geometry of fractures affects hydrogeochemistry	1,5 (High) Mineralogical composition, porosity, textural and structural anisotropy effects
2,1 (Low) Stress data affecting the geo-interpretation of fracture systems and rock mass	2,2 Rock Mechanics	2,3 (Medium) Spatial distribution of in situ stress and EDZ influences the hydrogeological regime	2,4 (High) Stress changes near fractures zones affecting flow may change precipitation	2,5 (Low) Rocks & fracture zones subjected to higher stresses may be more thermally conductive
3,1 (Medium) Hydrogeological tests and measures can affect the geo-interpretation of permeable features	3,2 (Medium) Water pressure changes the effective stress	3,3 Hydro-Geology	3,4 (Medium) The flow pattern affects dilution and mixing	3,5 (Low) The flow pattern will affect the temperature due to convection effects
4,1 (Low) Hydrogeochemistry interpretation affecting the interpretation of fracture min.rel.	4,2 (Medium) Precipitation in fractures affects the fracture stiffnesses, strengths and creep properties	4,3 (Medium) Effects of ground-water age, density, viscosity, and dissolution and precipitation	4,4 Hydro-geo-chemistry	4,5 (No effect)
5,1 (Medium) Thermal anisotropy and measurement affecting the geo-interpretation	5,2 (High) Change in temperature can change the local stress, possibly leading to failure	5,3 (Medium) Temperature gradients and thermal expansion in rock/fractures affect the water flow	5,4 (Medium) Dissolution and precipitation enhanced by thermal gradients	5,5 Thermal Properties

Fig. 4.1. Ranking the interactions in the off-diagonal boxes of the interaction matrix for their significance — as ‘no effect’, ‘low’, ‘medium’ and ‘high’.

4.2 Use of past experience in deciding on the couplings required in the numerical codes

Exploring the significance of THM couplings for repository performance has been a main theme of BENCHPAR WP2 to WP4 as these work packages were specifically set up to explore the significance of THM-processes for some PA-relevant issues. In order to obtain a structured input to these, a questionnaire was given to each Task Force leader of these work packages. The following questions were asked:

Q1

A: In what way is the work that you are doing relevant to making a safety case?

B: Are there performance measures to assess such relevance and, if so, what are they?

Q2

A: In terms of your Task, judge whether the individual couplings, TH, TM, HM, HT, MT, MH, are of High significance, Medium significance or Low significance.

B: Explain how and why the 'High significance' couplings affect the THM processes.

Q3

A: What are the main uncertainties in your work?

B: Are you able to assess these uncertainties in relation to other uncertainties, including the spatial uncertainty of rock properties.

These questions were subsequently discussed between the different modelling teams and also at several BENCHPAR workshops. The resulting judgements have already been summarised in Tables 3.1 to 3.3 in Section 3.

5 Technical Auditing of THM Numerical Analyses

5.1 The need for technical auditing of THM numerical analyses

The term 'technical auditing' (TA) means examining the technical content of a THM numerical analysis to establish if it is adequate for the purpose. The reason for requiring such a capability is that, in order to be able to coherently design a repository in a rock mass and conduct PA analyses, one must be able to predict the consequences of different design options. It is anticipated that the main method of developing this predictive capability is to use THM numerical modelling techniques. However, there are problems relating to such modelling — in terms of ensuring that all the relevant variables, parameters and mechanisms have been included in the modelling and that the model does represent the rock reality.

Questions have to be asked relating to the generation of the modelling output. Examples of such questions are listed below.

What is the work/project objective?

Have the relevant variables & mechanisms been identified?

Is the model/code adequate?

Which data are required?

How should the data be obtained?

Are the data adequate?

Has the model been used properly?

What are the prediction/back analysis protocols?

The basic modelling requirements can be seen from Fig 5.1. This diagram indicates that, for modelling the underground environment, it is necessary to include the rock mass geometry, the in-situ rock stress, the properties of the intact rock and fractures (or discontinuities), the hydrogeology and the excavation process. Depending on the analysis objective, other factors may also need to be included, e.g. thermal processes, geochemical processes, time-dependent processes.

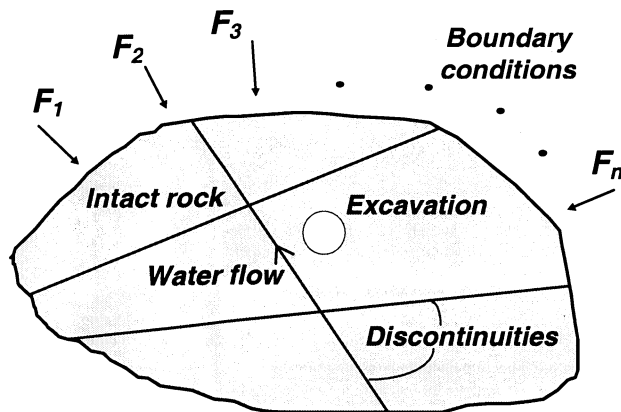


Fig. 5.1. The repository modelling problem. The boundary conditions (here indicated by the forces, F_i) are usually taken as the in-situ rock stress values, but there are also thermal and hydrogeological boundary conditions.

5.2 The technical auditing approach

There are different ways of conducting a technical audit. For example, a 'soft audit' enables the features of the modelling to be established and statements made concerning whether the right approach has been adopted in principle. Alternatively, a 'hard audit' involves a detailed analysis of the modelling to establish the relevant variables, mechanisms and parameters, whether the modelling is relevant and whether the design is appropriate and robust.

There are also other issues related to scientific consensus — because there are still many unresolved issues in engineering geology, rock mechanics and modelling. The review paper by Jing & Hudson (2002) provides an overview of the current status of numerical modelling. Issues of special difficulty and importance are the following.

Systematic evaluation of geological and engineering uncertainties.

Understanding and mathematical representation of large rock fractures.

of fracture shape, size, connectivity and effect of fracture intersections for DFN and DEM models.

Representation of rock mass properties and behaviour as an equivalent continuum and existence of the Representative Elemental Volume (REV).

Representation of interface behaviour.

effects, homogenization and upscaling methods.

representation of engineering processes, such as excavation sequence, grouting and reinforcement.

Time effects.

Large-scale computational capacities.

Also, it has become clear that the most important step in numerical modelling is, not operating the computer code, but the earlier ‘conceptualization’ of the problem in terms of the dominant processes, properties, parameters and perturbations, and their mathematical presentations.

5.2 The ‘soft’ and ‘hard’ audits

The Soft Audit firstly establishes an overview of the THM modelling work and determines whether well-known issues of importance and difficulty in characterizing and modelling rock masses have been addressed at the outset. Then, the purpose, style, features and content of the modelling are listed so that they can be presented in a compact manner.

The Soft Audit thus has two parts:

Part 1: Establishing an overview of the modelling and whether it is robust, given the known difficulties of characterizing and modelling rock masses; and

Part 2: Establishing the modelling features, so that the modelling work can be compactly presented with an initial assessment of its adequacy.

For both parts, the audit is conducted through a suite of questions, the answers to which form an audit trail and enable the THM modelling work to be specified, justified and presented in a transparent manner.

5.2.1 Part 1 of the Soft Audit: ‘Robustness’ Questions

Establishing an overview of the modelling through a series of questions relating to rock mass modelling issues of special importance and difficulty.

In rock mass characterization and modelling, there are several well-known difficulties.

These difficulties do not have to be fully overcome in the THM modelling, but there should be adequate awareness of them. They should already have been addressed, at least in terms of explaining why the modelling is adequate given each difficulty. The robustness of the modelling approach is addressed through the suite of questions in Table 5.1.

Table 5.1. Questions relating to overviewing the modelling and considering how well-known difficulties in modelling rock masses have been addressed.

1. What is the purpose of the modelling?
2. In what way is this work different to previous similar modelling work?
3. What is the scale of the rock mass being modelled?
4. What is the basic modelling geometry?
5. Has it been necessary to divide the rock mass into separate rock mass domains ¹ ?
6. Are the intact rock properties being specifically incorporated?

¹ Rock mass domain: a region of the rock mass in which the rock properties are statistically similar, but different to the properties of the surrounding rock in other structural domains

7. How are the fracture properties being incorporated?
8. Are features of the structural geology of the rock mass being incorporated?
9. Are the rock mass properties being input directly (as opposed to being a result of the input intact rock and fracture properties)?
10. How have the rock properties been estimated?
11. Is a constitutive law required for the rock mass? If so, how was it established?
12. Has the rock mass been modelled as a CHILE ² material? What has been done to account for the DIANE ³ aspects of the rock reality?
13. How have the stress boundary conditions been established?
14. Does the model include any failure criteria. If so, which one(s)?
15. Is the rock being modelled as a continuum, discontinuum, or combination of the two?
16. What are the hydrogeological conditions in the modelling?
17. How have the hydrological boundary conditions been established?
18. Are effective stresses being used?
19. How are the thermal properties being incorporated?
20. How are the THM components being included in the modelling: as uncoupled components, pairwise coupled components, fully coupled components?
21. Are there any special boundary conditions, loading conditions, or rock mass features in the modelling?
22. Has physical rock testing been used to obtain the any parameters supporting the model?
23. Has there been any study of potential adverse interactions that could lead to positive feedbacks and hence instabilities — in the rock mass and in the modelling?
24. Have all the potential failure mechanisms been identified?
25. Have modelling sensitivity studies been undertaken?
26. Have modelling protocols been used?
27. How will the modelling methods and results be presented?
28. Can the modelling be verified/validated? — in this study and in principle?

² CHILE: Continuous, homogeneous, isotropic, linearly elastic

³ DIANE: Discontinuous, inhomogeneous, anisotropic, not elastic

29. Are there any features of the model or modelling work not covered by the points above?

5.2.2 Part 2 of the Soft Audit: Specifying the components and features of the modelling

The components and features of the model are then specified through a suite of questions. These are listed in Table 5.2 under the four subject areas of

- Modelling objective,
- Modelling concept,
- Modelling technique,
- Modelling adequacy.

Table 5.2: Soft auditing modelling specification and the associated questions.

<i>Auditing Component</i>	<i>Associated Questions</i>
Subject Area 1: Modelling Objective — Establishing the purpose of the work	
<p>1. THE MODELLING OBJECTIVE</p> <p>The purpose of the modelling?</p>	<p>1-1 Has the modelling objective been clearly established?</p> <p>1-2 How will it be known when the modelling work is completed?</p>
Subject Area 2: Modelling Concept — Describing the modelling concept and content	
<p>2. CONCEPTUALISATION OF THE PROCESSES BEING MODELLED</p> <p>The sub-system(s) being isolated for study. The physical processes involved.</p>	<p>2-1 What rock mass systems are being considered?</p> <p>2-2 What are the main physical processes being modelled?</p> <p>2-3 What is the changing independent variable?</p> <p>2-4 How is the system perturbed so that the mechanisms are initiated?</p>
<p>3. SPECIFICATION OF THE MODELLING CONTENT</p> <p>What are the physical variables, connecting relations, parameters, boundary conditions, initial conditions, etc.</p>	<p>3-1 Listing of the physical variables</p> <p>3-2 Listing of the THM couplings</p> <p>3-3 Is the model 1-D, 2-D, 3-D or some combination?</p> <p>3-4 Are you modelling a continuum or a discontinuum?</p> <p>3-5 Specification of the boundary conditions</p> <p>3-6 Specification of the initial conditions</p> <p>3-7 How is the final condition established?</p>
<p>4. MODELLING SOLUTION REQUIREMENTS</p> <p>What type of model output is required, given the stated modelling purpose?</p>	<p>4-1 What is the required model output?</p> <p>4-2 Does the model output match the modelling objectives?</p>

<p>5. MODELLING SOLUTION TECHNIQUE</p> <p>How is the required model output to be obtained?</p>	<p>5-1 In principle, how is the model output to be obtained: one code, one set of data, one run? – or a suite of numerical experiments?</p> <p>5-2 Are any quality control checks in place? Checking the input data have been entered correctly, validation against known solutions, independent duplication of runs?</p>
<p>Subject Area 3: Modelling Technique</p>	
<p>6. NUMERICAL CODE UTILIZED</p> <p>Which numerical code is to be used? How do we know that the code is operating correctly?</p>	<p>4-3 Which numerical code is to be used?</p> <p>4-4 Why is that code being used?</p> <p>4-5 Where did the code originate from?</p> <p>4-6 How has the code been validated?</p>
<p>7. SUPPORTING MODEL DATA & DATA INPUT METHOD</p> <p>What are the necessary supporting data? How are they to be obtained? How are they to be input?</p>	<p>7-1 Listing of type and justification of boundary conditions</p> <p>7-2 Listing of input data with source of the data and justification.</p> <p>7-3 Do the data have to be adjusted before being input?</p>
<p>8. MODEL SENSITIVITY ANALYSIS</p> <p>How does the model output depend on the model input in terms of whether a sensitivity analysis is required?</p>	<p>8-1 How does the model output depend on the input parameter values?</p> <p>8-2 Is a sensitivity analysis being conducted? If so, what type of analysis? Processes, mechanisms, parameters, boundary conditions, couplings, etc.</p> <p>8-3 How are the results of the sensitivity analysis to be summarized?</p>

<p>9. PRESENTATION OF MODELLING RESULTS</p> <p>Is it possible to demonstrate that the numerical code is operating correctly? Are the modelling results clearly presented?</p>	<p>9-1 Is it possible to demonstrate that the numerical code is operating correctly?</p> <p>9-2 Is it possible to show that the supporting data are reasonable assumptions for a rock mass?</p> <p>9-3 How are the modelling results to be presented?</p> <p>9-4 Does the presentation of the modelling results link with the modelling objective?</p>
<p>Subject Area 4: Modelling Adequacy</p>	
<p>10. SOURCES OF ERRORS</p> <p>What are the main sources of errors?</p>	<p>10-1 Have you already corrected any errors?</p> <p>10-2 List the sources of potentially significant errors.</p> <p>10-3 Do any of the potentially significant errors invalidate the modelling objective, concept and conclusions?</p>
<p>11. MODELLING ADEQUACY</p> <p>Does the modelling seem adequate for the purpose? Are there any problem areas? Is any corrective action required?</p>	<p>11-1 Do all the previous questions indicate that in principle the model is adequate for the purpose.</p> <p>11-2 If not, list the problem areas.</p> <p>11-3 What corrective action is required?</p> <p>11-4 Does the soft audit have to be repeated after corrective action has been taken?</p>

5.3 Developing the soft audit into the hard audit

The procedure for developing from the soft audit to the hard audit is shown in Fig. 5.2. The hard audit covers the same subject but requires detailed justification of the answers to the questions.

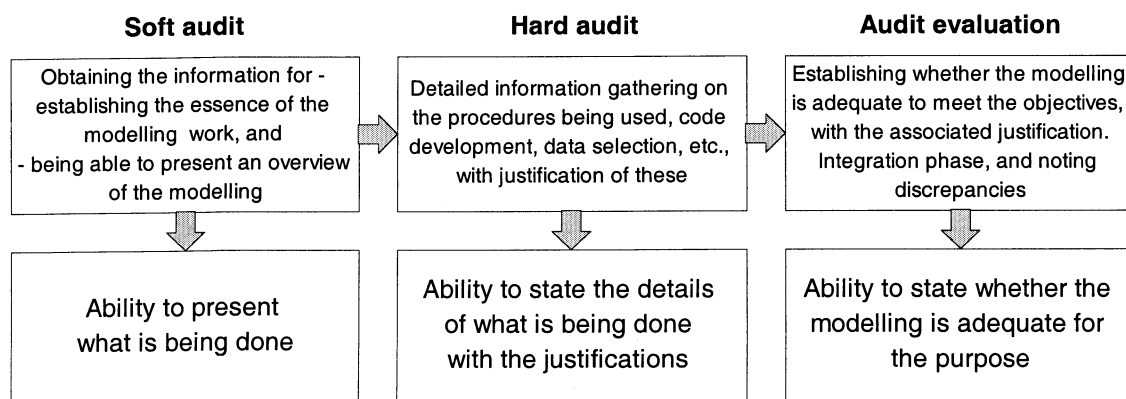


Fig. 5.2. The procedure for developing from the soft audit to the hard audit

It is important to note that it is not enough in the hard audit to say yes/no about the processes covered in the modelling: auditing work needs to cover the basic items of processes, equations, properties, parameters and methods. The hard audit results should be presented in the same form as the soft audit results, but including the necessary hard audit details and justifications.

5.4 Presentation of the auditing results

There should be clear presentations of the results. These can be in the form of a report or an effective alternative is a poster type display. Three types of presentation should be made.

What modelling work is being done or has been done in principle — the soft audit poster display.

What is being done and why it is being done in detail — the hard audit poster display.

Conclusions concerning whether the modelling is adequate for the purpose specified — the evaluation poster display.

These three reports or poster displays (with supporting documentation) are then suitable for communicating the modelling information, not only to geoscientists but to clients, disposers, regulators, managers and the public. The results ensure that the modelling is transparent and traceable through the audit trail.

6 Recommendations for THM analyses and Future Directions

6.1 Overview concluding comments

The BENCHPAR analyses, and especially Work Package 3 (Upscaling from the near-field to the far-field) show that uncertainty in analyses of flow in fractured hard rock formations stems from the following major sources of uncertainty:

- the characteristics of fractured media and the associated spatial variability; and
- the understanding of the nature and degree of coupling between rock mechanics and the hydraulic characteristics of fractures.

Developing a discrete fracture network (DFN) representation from a set of field data is far from elementary. Usually available data in terms of outcrop and borehole mapping, combined with hydraulic tests in boreholes, leave considerable ambiguity for the estimation of key DFN parameters such as fracture size permeability relations and fracture intensity. The analyses in Work Package 3 demonstrate that the resulting effective permeability of the rock mass may vary considerable depending on assumptions made in the data analysis. The uncertainties connected to this may be far larger than the uncertainties involved in describing the HM-MH couplings.

Also, the assumed coupling between fracture aperture and stress field directly affects the effective migration properties of the rock mass. In Work Package 3, differences between teams in using estimated effective permeability appear to depend essentially on whether the team used given apertures as input – and then calculated fracture transmissivity using the cubic law – or whether the hydraulic test data were used to calibrate the fracture transmissivity distribution.

6.2 Recommendations

In the light of the results presented, there are many implications for future work. However, the following recommendations are highlighted here concerning THM numerical modelling to support radioactive waste disposal.

- The problem set-up and data input can constitute major sources of uncertainty. It is recommended that the boundary conditions, problem geometry and rock properties are all carefully considered to avoid any ambiguities and misunderstandings.
- The stress-permeability relations are especially important and an effort should be made to ensure that these are well understood, particularly the influence of depth (and hence rock stress) on fracture permeability.
- It is the upscaling of hydraulic properties, rather than the added complication of T and M couplings, which is another main source of uncertainty. Thus, upscaling of rock mass effective properties in fractured hard rock formations is still a challenge and means to improve this are needed.
- Numerical modelling should include the most important coupled THM components and be followed by solute transport modelling.
- Sensitivity studies should be conducted to assess the significance of the different assumptions inherent in the problem idealization and rock property input values.
- The technical auditing procedure outlined in the document should be followed contemporaneously with the modelling as an on-going process since this is more efficient than solely post-modelling auditing.

6.3 Likely future directions

The future of the type of THM modelling described in this document depends on three main factors:

the PA/SA requirements for such modelling;

the ability of the software and hardware to be able to conduct the necessary modelling;

the ability to obtain realistic input for the modelling.

the ability to validate the results of the THM modelling.

It is likely that the requirement for the modelling will continue to be important not only for the transport modelling but also for the engineering design of a repository. At the same time the capabilities of software and hardware continue to increase year by year. However, the ability to obtain realistic input for the modelling is not likely to improve so quickly (see Jing, 2003, for a summary of the issues). Moreover, developing suitable validation procedures is particularly difficult. The site investigation procedures and testing in underground research laboratories can be enhanced, but the fundamental techniques and problems will remain very much the same.

Thus, the likely future directions are as follows.

Improvements in the numerical modelling leading to fully coupled codes.

The incorporation of coupled chemical processes in the THM codes.

The ability to incorporate more information in the problem configuration, e.g. more detailed rock fracture geometry.

More emphasis on obtaining realistic rock property input data.
More emphasis on validating the results of numerical codes through laboratory and in situ experiments.

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