SKB

TECHNICAL REPORT 93-12

Possible strategies for geoscientific classification for high-level waste repository site selection

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June 1993

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POSSIBLE STRATEGIES FOR GEOSCIENTIFIC CLASSIFICATION FOR HIGH-LEVEL WASTE REPOSITORY SITE SELECTION

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Information on SKB technical reports from 1977-1978 (TR 121), 1979 (TR 79-28), 1980 (TR 80-26), 1981 (TR 81-17), 1982 (TR 82-28), 1983 (TR 83-77), 1984 (TR 85-01), 1985 (TR 85-20), 1986 (TR 86-31), 1987 (TR 87-33), 1988 (TR 88-32), 1989 (TR 89-40), 1990 (TR 90-46) and 1991 (TR 91-64) is available through SKB.

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Keywords: Geostatistics, Siting of HLW, Geoscientific classification

ABSTRACT

This work was performed to suggest possible strategies for geoscientific classifications in the siting process of a high-level repository. To develop a feasible method for geoscientific classifications, a number of factors of a philosophical character, related to the purpose of the classifications, need to be accounted for. Many different approaches can be visualized, and this report was not intended to present a complete classification methodology. The purpose was rather to suggest some strategies for handling geoscientific factors that may be included and integrated in a functional classification methodology in the siting procedure. In this work it was assumed that geoscientific classifications will primarily be of interest with respect to the geoscientific aspects on the safety of the repository.

Before any geoscientific classifications can be performed, the following questions need to be addressed: what areas should be classified?; what methodology should be used?; and what parameters are of interest? To address these issues, the following parts are included in this report.

First, a strategy based on simple set theory was suggested to select areas suitable for geoscientific classifications. The areas are chosen with respect to the costs for the decisions related to each factor that is considered to be important. Possible factors are political, demographical, and economical factors.

Second, a strategy for classification of the geoscientific conditions was suggested based on the basic concepts of an American system for classification of groundwater vulnerability, DRASTIC. The suggested classification strategy has a so-called Bayesian approach, i.e. the classifications of the critical parameters are based on a combination of professional judgments and existing data. Due to limited economical resources, detailed investigations can never be performed to cover all areas that have to be included in the classification process and therefore the classifications have to some extent to be based on professional judgments. In the suggested strategy the critical parameters are treated stochastically and the classifications are updated as new data are collected.

Third, a selection of critical parameters to be included in the geoscientific classification was suggested, based on a literature review of geoscientific factors of importance to the safety of a repository. The parameters are related to the mechanical stability, transport of solutes, groundwater chemistry, groundwater flow, and the geological-structural setting.

Fourth, a simple test of handling a critical parameter in a Bayesian context was performed. RQD was used as the critical parameter. This approach allows for getting optimum value on a parameter from professional judgment and existing data. It also allows for estimations of where and to what extent new data should be collected, i.e it allows for decisions based on optimal use of the available information and knowledge at every stage of the siting process.

SAMMANFATTNING

Detta arbete genomfördes i avsikt att föreslå möjliga strategier för klassificering av geovetenskapliga faktorer i lokaliseringsprocessen av ett slutförvar. Det förutsätts att sådana klassificeringar i första hand kommer att vara intressanta med hänsyn till de geovetenskapliga aspekterna på säkerheten hos slutförvaret. Det är således inte avsikten att utveckla en klassificeringsmetodik som fullständigt beskriver de geologiska/hydrogeologiska förhållandena, utan snarare ser till kriterier som är av betydelse för slutförvarets säkerhet.

Innan några geovetenskapliga klassificeringar kan genomföras måste följande frågeställningar belysas: vilka områden skall klassificeras, vilka parametrar är relevanta för klassificeringarna och vilken metodik skall användas?

I denna rapport föreslås först en strategi för att välja områden som skall klassificeras. För en kostnadseffektiv valprocess identifieras dessa områden med hänsyn till kostnaderna för de beslut som måste tas för relevanta faktorer. Sådana faktorer kan vara politiska, befolkningsmässiga och ekonomiska.

Därefter föreslås en strategi för den geovetenskapliga klassificeringen, utgående från de grundläggande elementen i DRASTIC, ett amerikanskt system för klassificering av grunvattnets sårbarhet. Den föreslagna klassificeringsmetodiken har ett s k Bayesianskt angreppssätt, dvs klassificeringarna baseras på en kombination av befintliga data och erfarenhetsmässiga bedömningar. På grund av begränsade resurser kan detaljerade undersökningar aldrig genomföras heltäckande för de områden som skall inkluderas i klassificeringarna, vilka därför till viss del måste baseras på erfarenhetsmässiga bedömningar. I den föreslagna metodiken hanteras de kritiska parametrarna stokastiskt och klassificeringarna uppdateras så snart nya data blir tillgängliga.

Som en tredje del i detta arbete föreslås en uppsättning kritiska parametrar för de geovetenskapliga klassificeringarna. Förslagen till de kritiska parametrarna baseras på en litteraturgenomgång av faktorer viktiga för slutförvarets säkerhet. Parametrarna är valda med avsikt på mekanisk stabilitet, föroreningstransport, grundvattenkemi, grundvattenflöde och strukturgeologi.

Den fjärde och sista delen behandlar hantering av de kritiska parametrarna med ett Bayesianskt angreppssätt. För att exemplifiera detta angreppssätt valdes RQD som en kritisk parameter och resultaten indikerar att en sådan hantering kan ge optimal information om en parameter utifrån erfarenhetsmässiga bedömningar och befintliga data. Det Bayesianska angreppssättet möjliggör också bedömningar om var och i vilken omfattning nya data skall inhämtas, vilket innebär att besluten på respektive nivå i lokaliseringsprocessen kan göras utifrån optimalt utnyttjande av den tillgängliga geovetenskapliga informationen och kunskapen.

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1 INTRODUCTION

The predominant process for transport of radionuclides into the biosphere from a high-level waste repository at large depths in crystalline rocks, is groundwater movement. The conditions for groundwater movement depend on a number of geological, hydrogeological, and geochemical factors and there has been a vast amount of research performed to study these factors at repository depths. Canada, Sweden, and Switzerland have extensive research programs aiming at assessing the long term safety of nuclear waste repositories in crystalline rocks. Several other countries, e.g. USA, Great Britain, Japan, and France, have or have had research programs dealing with nuclear waste repositories in crystalline rocks. The main purpose of these programs is to understand in detail the specific processes that determine the conditions for radionuclide transport in fractured media.

However, in the process of repository siting there are economical limitations and the search area is initially large, probably an entire country. It is therefore not possible to perform detailed geoscientific investigations of the entire search area. Detailed studies have to be restricted to small areas and specific sites, which should be chosen with respect to political, social, economical, geoscientific, and other factors considered important. To implement a credible siting process, a clear and straightforward strategy should be applied to identify areas and sites for detailed investigations with respect to important factors. A tool for handling the geoscientific part of this strategy may be a classification methodology that integrates existing knowledge and geoscientific information, such as geological maps, topographic maps, satellite imagery, and well-logs.

Compared to the research efforts oriented towards safety assessments and detailed understanding of transport processes, little emphasis is being put on how to use already existing geoscientific information and how to correlate that information to the present understanding of the transport and safety conditions at repository depths. To perform geoscientific classifications in areas where no detailed investigations have been made, such knowledge is, however, of primary importance.

This work was performed to suggest some possible strategies for how to handle geoscientific issues in the siting process that may be relevant to include and integrate into a classification methodology.

The following issues were addressed:

1. **The selection of areas for geoscientific classification.** Due to political, demographic, economical, and other non-geoscientific factors, several areas are not suitable for a repository and should be excluded from the classification process.

2. **The classification approach.** Because of the ever present geoscientific uncertainties, the classification methodology should allow for a proper handling of these uncertainties and be able to make optimum use of existing knowledge and data.

3. **The critical parameters to be included in the classifications.** The classification method should include parameters that properly describe and predict present and future geoscientific conditions, primarily with respect to the safety and performance of the repository.

The purpose of this work was to:

1. Suggest a strategy to identify areas for geoscientific classifications.

2. Suggest a strategy for geoscientific classification.

3. Discuss possible critical parameters to be included in the geoscientific classification methodology.

4. Perform a pilot-test of classification of a parameter using a combination of professional judgment and existing data.

2 A STRATEGY FOR IDENTIFICATION OF AREAS FOR GEOSCIENTIFIC CLASSIFICATION

2.1 INTRODUCTION

The strategy discussed here for identification of areas of interest for geoscientific classifications, is based on the costs for the decisions related to each factor considered to be of importance. It is assumed that by making decisions in sequence with respect to increasing costs, starting with the least expensive decisions, unsuitable areas can be discriminated in a cost-effective way. Within the scope of this work, it was only possible to discuss a possible strategy to handle the decisions cost-effectively, and not to analyze the costs for specific decisions.

2.2 IDENTIFICATION STRATEGY

Initially, the search area for finding a suitable location for the repository will be the entire Sweden (figure 2.1).

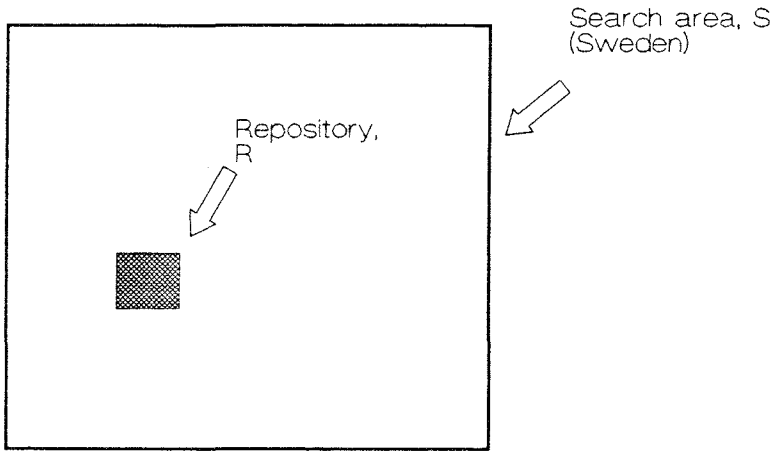

Figure 2.1. Search area for siting of repository.

It is assumed here that for a certain cost, C_i, all conditions can be completely understood within a certain area, A, so that the waste can be properly disposed with respect to the factor i. It is also assumed that the costs for evaluating i are proportional to the area, so that

$$C_i = c_i A_i \qquad (2.1)$$

The factors i may be:

p	political
f	demographic
e	economical
g	geoscientific

If all conditions are completely understood a suitable area for the repository, A_i, can be identified with respect to the factor i. However, when dealing with high-level radioactive wastes, it may from a psychological point of view be more appropriate to find the complementary to A_i, i.e. where it is <u>not</u> suitable to site the repository. The complementary is:

$$A_i^C = S - A_i \qquad (2.2)$$

where S is the entire search area, i.e. Sweden in this case.

To perform a cost-effective siting process, the main objective would be to find:

$$MIN\ [\ \sum_i c_i(A_i\ alt\ A_i^C)\ ] \qquad (2.3)$$

With respect to the factors mentioned above, i.e. political, demographic, economical, and geoscientific, a suitable repository, R, can be sited using simple set theory:

$$R = A_p \cap A_f \cap A_e \cap A_g = \bigcap_i A_i \qquad (2.4)$$

The complementary to A_i can also be used to site R:

$$R = \bigcap_i (S - A_i^C) \qquad (2.5)$$

The repository suitable site is shown in figure 2.2.

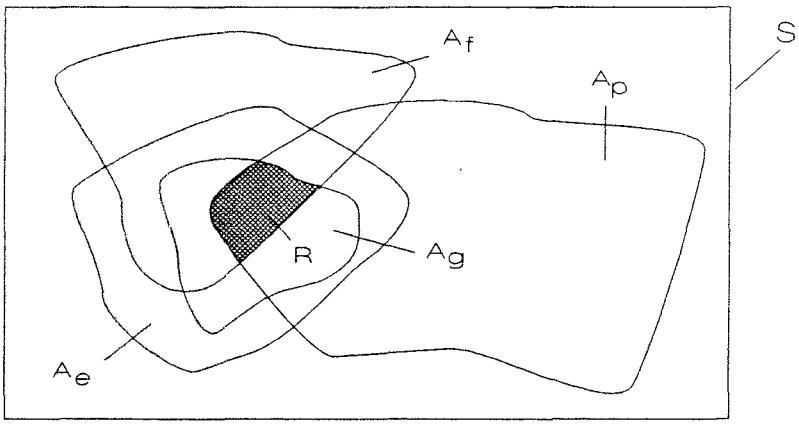

Figure 2.2. The suitable repository site.

The assumption that all factors are completely understood makes it possible to treat the factors as independent sets of information and to:

1. Beforehand choose whether to determine A_i or A_i^C

2. Determine A_i or A_i^C with respect to the factors i in an arbitrary order.

This allows for making decisions in sequence with respect to increasing costs, starting with the least expensive decisions. This approach can give a cost-effective identification of a suitable repository area. Given the above mentioned factors, it may be assumed that:

$$c_p < c_f < c_e << c_g$$

A political decision does not, at least directly, imply any costs, population statistics are already available, economical decisions are mainly related to transport distance, and geoscientific studies are by comparison very resource demanding. It should be emphasized that several levels of geoscientific decisions can be visualized, e.g (1) very early assessments, e.g to avoid the Fennoscandian mountain range and ore deposits of Bergslagen; (2) those related to analysis of existing information to achieve a basis for further detailed studies; and (3) those related to detailed studies. The first type of geoscientific decisions may be included in the political decisions, whereas the last two types are much more expensive. If the last two types are looked upon collectively they will probably be the most expensive decisions taken in the siting process.

Since it from a psychological point of view may be advantageous to determine A_i^c:s rather than A_i:s, the complementaries should be used to the greatest extent. When an unsuitable area for the repository, A_i^c, has been identified with respect to one specific factor, no further studies need to be performed with respect to other factors in that area. This means that for all other factors than the first one, it is not necessary to know everything for the entire search area (Sweden). *For a specific factor everything has to be understood only for the area that has not been previously discriminated.*

However, when dealing with the geoscientific part of the process, it will, due to geologic complexities and economical limitations, be impossible to completely understand all conditions for all areas that has not been discriminated by the other factors. The geoscientific classification strategy described in chapter 3 is intended for handling of the uncertainties resulting from this incomplete understanding. It is, with respect to the geologic environment and the classification strategy, appropriate to determine A_g instead of the complementary, A_g^c. This means that the strategy to find a repository would be modified and defined as:

$$R = A_g \cap [\bigcap_j (S - A_j^c)] \qquad (2.6)$$

where j are all non-geoscientific factors.

The idea of performing geoscientific classifications is to reach an initially high plateau of knowledge for directing detailed studies to interesting sites. The decisions associated with the classifications are probably rather resource demanding compared to those related to factors such as politics, economy, and population. Classifications may therefore be performed just before the detailed geoscientific studies. In analogy with the above reasoning, areas of interest for geoscientific classifications can be identified by a sequential handling of non-geoscientific factors:

$$G = \bigcap_j (S - A_j^c) \qquad (2.7)$$

where G is the area for geoscientific classifications. The strategy for finding a areas for geoscientific classifications is schematically described in figure 2.3.

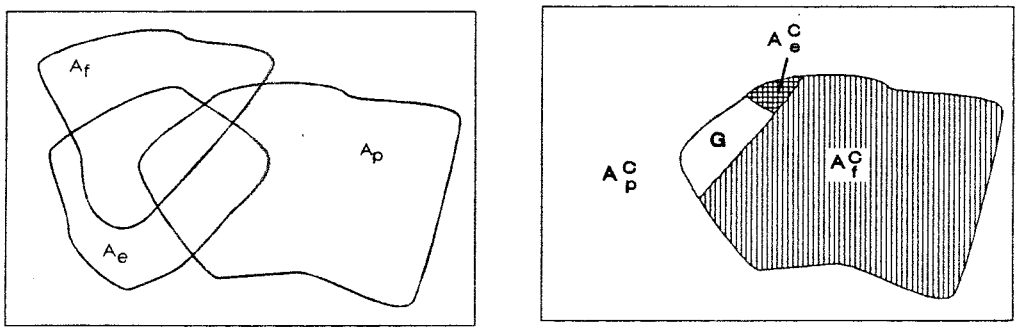

Figure 2.3 Conceptual description of area discrimination for geoscientific classification. In this example decisions are made in the following order: (1) political, (2) demographic, and (3) economical.

2.3 DISCUSSION

In the siting process of a high-level waste repository, it is from a psychological point of view suggested that unsuitable areas, rather than suitable, for the repository are delineated. For many siting factors it should be easier to defend a discrimination of an unsuitable area rather than an identification of a suitable one, probably more so for political and demographical factors than economical ones.

To identify areas that are of interest for geoscientific classifications in a cost-effective way, it is suggested that decisions are made in sequence with respect to increasing costs, starting with the least expensive costs. The suggested strategy for identification of suitable areas for geoscientific classification can be summarized as:

1. Determine the sequence for the decisions to be made.

2. Identify areas for geoscientific classifications using the suggested identification methodology.

3. Perform geoscientific classification.

3 A STRATEGY FOR A GEOSCIENTIFIC CLASSIFICATION METHOD

3.1 INTRODUCTION

There is a strong intuitive aversion against any kind of waste-disposal in our close proximity, commonly referred to as NIMBY (Not In My Backyard). If geoscientific classifications are included as a part of the siting process of a high-level repository, a classification strategy that is logical and straightforward should be applied. The basic concepts of two standardized systems for classification of groundwater vulnerability and risk assessments, DRASTIC (Aller et al, 1987) and the LeGrand-system (LeGrand, 1983) respectively, have been used to good advantage in the siting process of waste-disposal sites in Sweden (Holmstrand and Svensson, 1988). The approach of these methods is to provide qualitative guidelines on a principal level, i.e they focus on ***criteria*** that should be considered rather than specific, or unique, conditions at each site or area. Similar systems are widely used in other fields, e.g. Barton's Q-value (Barton et al, 1974) and the RMR-method (Bieniawski, 1979) in rock-mechanics.

In this section the possibilities for using the basic concepts of this type of classification system for geoscientific classification in the repository siting process are discussed. The purpose was (1) to describe the statistical properties of such systems; (2) to introduce uncertainty estimations and updating in these systems; and (3) to discuss a conceptual classification strategy for siting of sites of a repository. DRASTIC and the LeGrand-system are similar in many respects but DRASTIC has been chosen as a starting point for this study, since it is more suited for regional analysis than the LeGrand-system. The main part of this chapter was earlier published by Rosen and Gustafson (1992).

3.2 GENERAL DESCRIPTION OF DRASTIC

DRASTIC uses a set of seven hydrogeologic key parameters to classify the relative vulnerability to contamination of an aquifer:

D Depth to Groundwater
R Recharge
A Aquifer Media
S Soil Media
T Topography
I Impact of the Vadose Zone Media
C Conductivity (Hydraulic) of the Aquifer

The parameters are weighted between 1 and 5 with respect to their relative importance for the vulnerability of the aquifer. Depth to Groundwater and Impact of the Vadose Zone Media are considered to be the most important factors and have a weight of 5 while Topography is the least important with a weight of 1. Each parameter has a rating between 1 and 10 with respect to the actual value of the parameter. The ratings for Depth to Groundwater are listed in table 3.1.

Table 3.1. Ratings of Depth to Groundwater in DRASTIC.

Depth (meters)	**Rating**
0-1,5	10
1,5-4,5	9
4,5-9	7
9-15	5
15-23	3
23-30	2
> 30	1

A DRASTIC-index is calculated for an area by:

$$D_W D_R + R_W R_R + A_W A_R + S_W S_R + T_W T_R + I_W I_R + C_W C_R =$$

$$= \textit{DRASTIC-index}, \qquad (3.1)$$

where W = Weight and R = Rating. The higher DRASTIC-index, the higher the relative groundwater vulnerability.

DRASTIC assumes that (1) the contaminant is introduced at the ground surface; (2) the contaminant is flushed into the groundwater by precipitation; (3) the contaminant has the mobility of water; and (4) the area evaluated using DRASTIC is 100 acres or larger.

3.3 STATISTICAL DESCRIPTION OF DRASTIC AND SIMILAR SYSTEMS

DRASTIC and the LeGrand-system have statistical properties that are not explicitly displayed in the manuals to the systems but have been indicated by Rosén (1991). The index-rating methodology in DRASTIC and similar systems can be described as a multiattribute utility function, which has the principal form (USDOE, 1985):

$$u(x_1,\ldots,x_n) = f[u_1(x_1),\ldots,u_n(x_n)], \qquad (3.2)$$

where, specifically for DRASTIC, the DRASTIC-index, u, is a function of a set of critical parameters, x_i $(i = 1,\ldots,n)$. The assessment of u can be divided into parts where the function for each part, or critical parameter, u_i $(i = 1,\ldots,n)$, is easier to handle than the vulnerability as a whole.

The multivariate utility function is an objective function that can provide a relative ranking of the consequences from a certain activity by assigning a value, or rating, to each consequence. Conceptually, the ratings of the critical parameters describe what are the specific impacts from a polluting activity, whereas the indices describe the total effects or consequences of those impacts in relative terms.

The classification procedure in DRASTIC and similar rating systems can also be described in another way with respect to the components of the systems:

$$\begin{bmatrix} T_{11} & .. & .. & .. \\ .. & .. & .. & .. \\ .. & .. & .. & .. \\ .. & .. & .. & T_{NM} \end{bmatrix} \begin{bmatrix} A_1 \\ .. \\ .. \\ A_N \end{bmatrix} = \begin{bmatrix} C_1 \\ .. \\ .. \\ C_M \end{bmatrix} \qquad (3.3)$$

$$\begin{bmatrix} W_{11} & .. & .. & .. \\ .. & .. & .. & .. \\ .. & .. & .. & .. \\ .. & .. & .. & W_{KM} \end{bmatrix} \begin{bmatrix} C_1 \\ .. \\ .. \\ C_M \end{bmatrix} = \begin{bmatrix} I_1 \\ .. \\ .. \\ I_K \end{bmatrix} \qquad (3.4)$$

where ^{o}T are the transformation operations, e.g. different kinds of modeling and analysis, that are performed on sets of data, A, to obtain values of the critical parameters, C.

Assets, or data sets *(A:s)* may be geological maps, well-logs, results from pumping tests, etc. A transformation operation *(T)* might be an analysis of hydraulic conductivity distributions in an area from pumping tests *(A:s)*, if hydraulic conductivity is a critical parameter *(C)*. The transformation operations may be subject to updating as new sets of data become available. For example, as additional pumping tests are performed in the area, a new transformational operation can be performed to update the hydraulic conductivity distribution.

In expression (3.4) the critical parameters *(C:s)* are related to each other with respect to their relative importance using weight functions *(W:s)* for each parameter. The simplest form of a weight function is a constant, as in DRASTIC. One parameter can have different weight functions (between 1 and K), as described by the weight matrix, with respect to the purpose of the classification. For example, to predict the behavior of pollutants in the ground, the importance, or weight, of each critical parameter may vary with the type of pollutant. The critical parameters and the weights produce an index, I, that is a relative value of the evaluation.

The critical parameters and their relative weights in DRASTIC have been chosen through consensus using a so called delphi-approach. This technique is commonly used to reach decision when data are too sparse for quantitative validations.

Some more specific features in DRASTIC, in addition to the general description above, should also be pointed out. DRASTIC has as many as seven correlated critical parameters. The higher the number of parameters, the lower the coefficient of variation of the results from different evaluators, since the standard deviations of the parameters are subject to vector addition. Also, since several parameters in DRASTIC are correlated, there is a redundance effect that tends to decrease the impact of misjudgments of individual parameters, provided that they are treated individually (Rosén, 1991).

3.4 UNCERTAINTY ESTIMATIONS AND UPDATING

Every geoscientific evaluation is associated with uncertainties that may be reduced but never completely eliminated due to heterogeneous and complex geological conditions. To introduce uncertainty estimations of the results into this type of classification systems, we need to go from the qualitative-guideline approach towards a more quantitative, stochastic approach. In a stochastic model each parameter is treated as a probability distribution function *(PDF)* as opposed to a deterministic model where each parameter has a specific, absolute value. Uncertainty estimations allow for updating of the results as new data become available. In the updating process, the following issues are of primary importance: (1) the worth of existing data and (2) the amount of new data that is needed to reach a specific confidence level for the evaluation.

For uncertainty estimations and updating in a system for hydrogeological classification a Bayesian approach is suggested. Bayesian statistics differ from classical statistics by not requiring that the probability distributions are based on measured data. With a Bayesian approach, the *PDF* can be based on limited data or on professional judgments from past experiences, even before any measurements are taken. This allows statistical handling of a parameter also if data are sparse or absent, which is many times the case for geological and hydrogeological parameters, e.g. porosity and hydraulic conductivity.

The Bayesian statistics can be described as:

$$P[A_i \mid B] = P[A_i]\{additional\ knowledge\} \tag{3.5}$$

which indicates how the *prior* probabilities estimated before an experiment, A_i $(i = 1,\ldots,n)$, should be modified by the evidence of a new outcome, B, to produce *posterior* probabilities.

The prior estimation of A_i can be based on professional judgment from past experiences only, or on experience and existing data. As new data become available the estimation of the PDF is updated to a higher degree of certainty, or a posterior estimate. Updating can be performed every time additional data become available. For every updating the uncertainty is estimated. When data are sparse, the Bayesian statistical estimates might be quite different from classical statistical estimates of the same dataset but as additional data become available the two different types of estimates converge. Figure 3.2 gives a general description of the Bayesian Updating process. Bayesian statistics in hydrogeology have been described by Massmann and Freeze (1987) and Freeze et al (1990) among others.

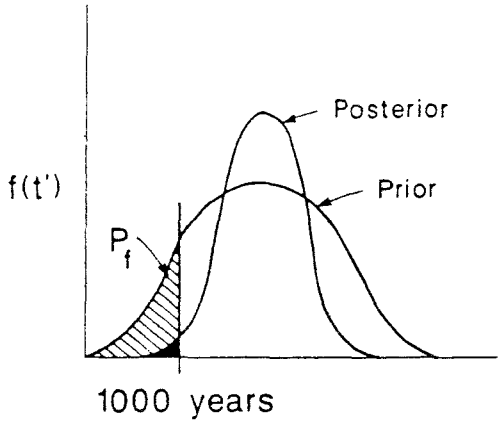

Figure 3.2. Bayesian updating of a time-related parameter with prior and posterior PDF showing reduction in probability of failure, P_f, from prior to posterior (after Freeze et al, 1990).

3.5 A CONCEPTUAL CLASSIFICATION STRATEGY

In order to develop a system for siting of high-level radioactive waste-disposal with respect to geoscientific conditions, a number of geological and hydrogeological parameters need to be considered. The United States Department of Energy (US-DOE, 1985 and 1986) has within the repository program in USA suggested that a decision framework has to be applied to handle such a variety of information properly. Freeze at al (1990) described the application of decision analysis in hydrogeological evaluations.

In the previous sections it was described how DRASTIC and similar systems are developed in order to integrate critical parameters of various importance. It has also been suggested that uncertainty estimations and updating are included in the classification methodology to assess (1) the worth of existing data and (2) the amount of new data that is needed to reach an acceptable confidence level for the evaluation. Such a basic structure may be a possible way for a build-up of a suitable classification methodology.

The ultimate objective of the geoscientific classifications will be to find areas where the hydrogeological conditions are favorable so that transport of radionuclides at a certain concentration beyond a certain compliance boundary is not allowed. The compliance boundary of primary interest at this stage of the siting process may be between the hydrogeological environment and the biosphere. The introduction of the pollutant from the repository, its barriers, and the near-zone into the undisturbed hydrogeologic environment may be described as a step function, shown in figure 3.3.

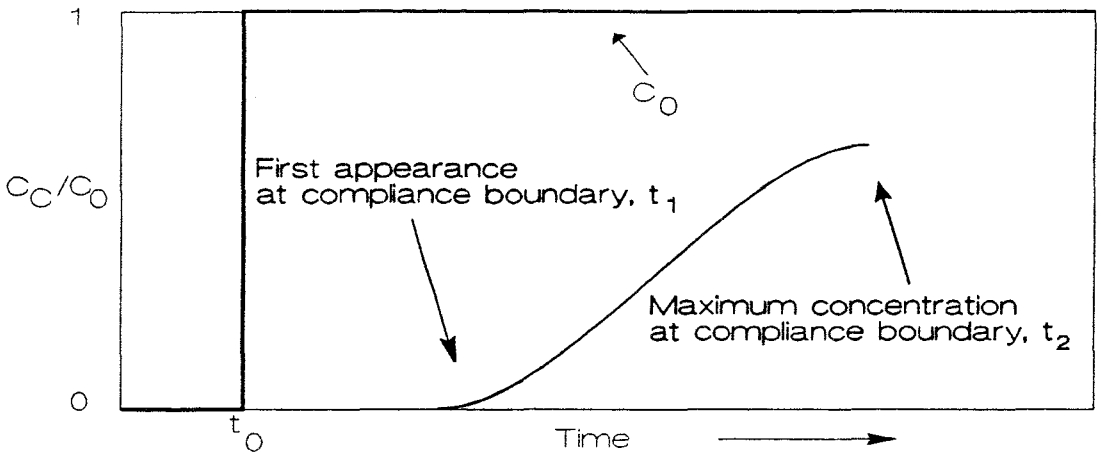

Figure 3.3. Step function describing continuous supply, C_0, of the radioactive pollutant after time t_0 into the hydrogeologic environment, its first appearance at the compliance boundary (the biosphere) at time t_1, and the maximum concentration reaching the compliance boundary at time t_2.

If it is assumed that the pollutant is subject to exponential degradation, the concentration reaching the compliance boundary, i.e. the biosphere, can be described by the following expressions:

$$C_C = 0 \quad for \quad t \leq t_0 \prod_{i=1}^{N} \theta_i \qquad (3.6)$$

$$C_C \leq C_0 e^{-\lambda t} \prod_{i=1}^{n} \Sigma_i \quad for\ all\ t \qquad (3.7)$$

where C_0 is the concentration entering the hydrogeologic environment at t_0 and C_C is the concentration reaching the compliance boundary for the first time at t_1 and its maximum level at t_2. λ is the radioactive decay constant. Σ_i and θ_i are sets of reduction and retardation factors, which can be regarded as critical parameters to describe the potential for the pollutant reaching the biosphere.

Among the critical parameters, in addition to the initial concentration entering the hydrogeologic environment, may be: (1) sorptive capacities of the geologic material; (2) the travel time through the hydrogeologic environment; and (3) geochemical properties such as oxidation-reduction.

Since all critical parameters, Σ_i and θ_i are associated with uncertainties, it should be attempted to estimate (1) what amount of new measurements are needed to decrease the uncertainty and (2) where, i.e. for what parameters and on what locations, are new measurements most valuable. The classification procedure may thus provide suitable data for a decision analysis of both site selection and further measurements.

When treating the critical parameters as probabilities, as opposed to fixed ratings in DRASTIC and similar systems, the conceptual model for the classification procedure will become:

$$\begin{bmatrix} T_{11} & .. & .. & .. \\ .. & .. & .. & .. \\ .. & .. & .. & .. \\ .. & .. & .. & T_{NM} \end{bmatrix} \begin{bmatrix} A_1 \\ .. \\ .. \\ A_N \end{bmatrix} = \begin{bmatrix} P(\Theta_1,\Sigma_1) \\ .. \\ .. \\ P(\Theta_M,\Sigma_M) \end{bmatrix} \tag{3.8}$$

$$\begin{bmatrix} W_{11} & .. & .. & .. \\ .. & .. & .. & .. \\ .. & .. & .. & .. \\ .. & .. & .. & W_{KM} \end{bmatrix} \begin{bmatrix} P(\Theta_1,\Sigma_1) \\ .. \\ .. \\ P(\Theta_M,\Sigma_M) \end{bmatrix} = \begin{bmatrix} P(R_1) \\ .. \\ .. \\ P(R_K) \end{bmatrix} \tag{3.9}$$

where T are the transformations, A are the data sets, P are the probabilities for the critical parameters θ and Σ, and R are the classification results. Several parameters may be associated with very high uncertainties in the first stages of a site-screening process. It is, however, suggested that all parameters considered to be critical are included in all stages throughout the classification procedure in order to defend the siting process. It may not be appropriate to alter the criteria for siting after one or more stages of the process have been performed. The Bayesian approach suggested here allows for estimations based on professional experiences where data are sparse, and is therefore of primary importance to make decisions regarding further actions possible. Such decisions may be regarding where and to what extent new data should be gathered.

3.6 DISCUSSION

It has been suggested that the basic properties of DRASTIC and similar classification systems are used for geoscientific classifications in the siting process of high-level nuclear wastes. The overall purpose of the suggested strategy is to take into account the uncertainties of the geoscientific environment and to allow for decision analysis at every stage of the classification. The system should be applied not only in the first screening of large areas, based on existing data and professional judgments, but also in more detailed studies, to a larger extent based on measurements.

4 CRITICAL PARAMETERS FOR GEOSCIENTIFIC CLASSIFICATION

4.1 INTRODUCTION

To perform the classifications of the geoscientific conditions for a high-level radioactive waste repository in accordance to the strategy suggested in chapter 3, a set of critical parameters have to be selected. This chapter is a literature review of factors that may be of interest to include in the classification methodology, with special emphasis on safety factors.

The following issues were studied in the preinvestigations at the Äspö Hard Rock Laboratory (HRL) and are, according to Gustafson et al (1991), key issues in geoscientific predictions on every scale, regional as well as site specific:

* The geological-structural setting
* Groundwater flow
* Groundwater chemistry
* Transport of solutes
* Mechanical stability

The possibilities for taking these issues into account in the suggested classification strategy are discussed in this chapter. The purpose is to suggest parameters that may be critical to describe these key issues and that are possible to assess with some degree of confidence from existing knowledge and data. The above mentioned issues are discussed with respect undisturbed conditions, i.e. conditions that will exist in the far-zone. For every parameter that is suggested in the following sections, a strategy for how to perform estimations prior to detailed investigations is discussed.

Since the preinvestigations at the Äspö HRL were similar to the suggested classification strategy in some respect, with predictions based on experiences before detailed studies were performed, that work has been of great importance for the reasoning in the following sections. A major difference between the Äspö preinvestigations and the classification process is that the former were aimed at understanding processes, whereas the latter is performed mainly with respect to the repository establishment. However, both kinds of assessments are restricted to the same information and the results and experiences from the Äspö HRL are therefore considered to be of great value to the classification process.

4.2 RESOLUTION AND VALIDITY SCALES

The objective of the geoscientific classification is to find areas of interest for detailed investigations for repository construction. The magnitude of the repository is in the order of 10^3 meters. This means that the classifications should be valid for areas corresponding to this magnitude. To achieve this validity, the resolution of the classifications should be higher than the repository magnitude. A measure of a realistic resolution may be the Representative Elementary Volume (REV).

REV is a measure of the smallest volume where the medium can be treated as homogeneous for spatial scales with respect to a specific factor, e.g. hydraulic conductivity. For conductivity measurements the REV must include a sufficient number of pores or fractures to permit a meaningful statistical average required in a continuum approach (Freeze and Cherry, 1979). The relation between the REV and a geologic parameter, porosity, is displayed in figure 4.1.

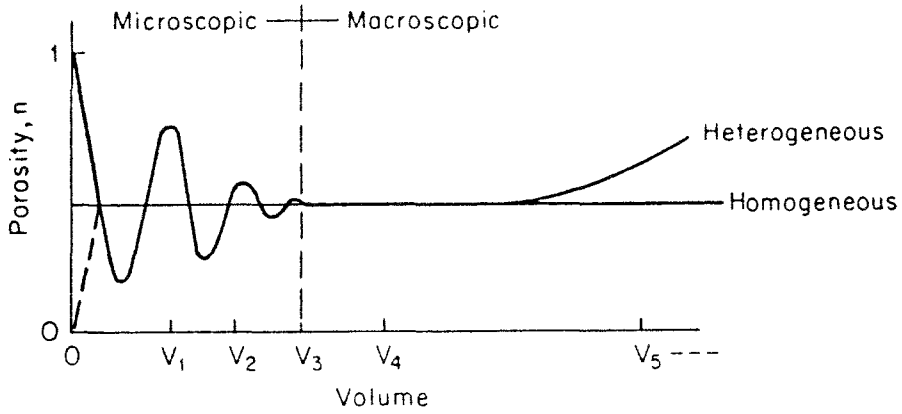

Figure 4.1. Possible relation between porosity and the representative elementary volume (REV) of a geologic medium (from Freeze and Cherry, 1979, after Hubbert, 1956; Bear, 1972). The right end of the curve is due to megascopic, or regional, heterogeneities.

REV is thus regarded as the resolution of the geoscientific classification. For crystalline rocks, REV may have a magnitude of 10^2 meters with respect to some parameters, e.g. hydraulic conductivity on the large scale. Throughout this chapter, the handling and values of parameters refer to assessments that can be carried out on a larger rock volume than the REV. It should be pointed out that the REV may be different for different parameters and that it is not clear that an REV can be designated to every parameter. However, for classification purposes the REV is still a useful measure, to which estimations to the greatest extent possible should be valid in order to obtain relevant classification results.

The classified area, on the other hand, should be considerably larger than the repository to make a meaningful classification. A realistic assumption may be that every classified area should be at least 10 times larger than the repository, i.e. have a magnitude of 10^4 meters. This corresponds very well to the scales used for the investigations at the Äspö HRL (figure 4.2).

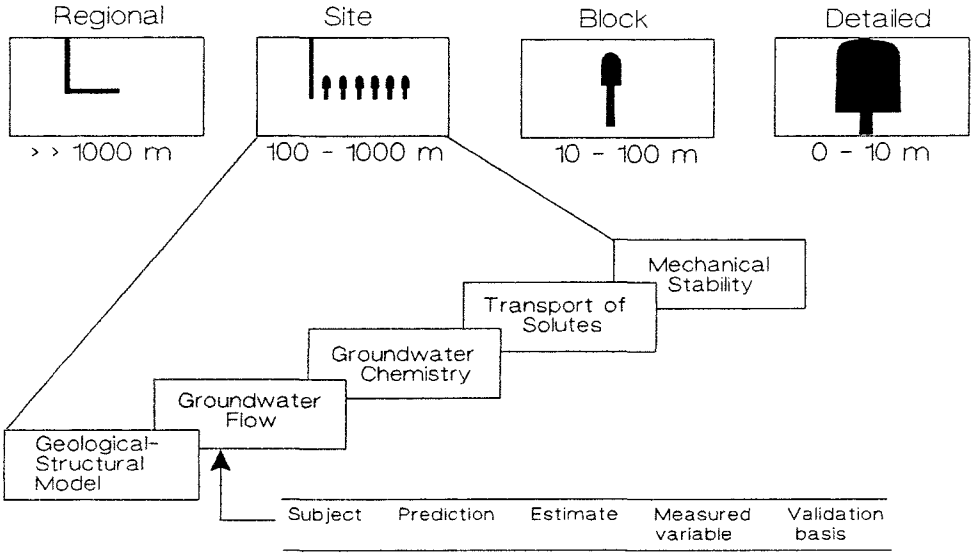

Figure 4.2. Overview of issues and investigation scales at the Äspö HRL (Gustafson et al, 1991).

The scales and issues for the geoscientific classification is schematically described in figure 4.3.

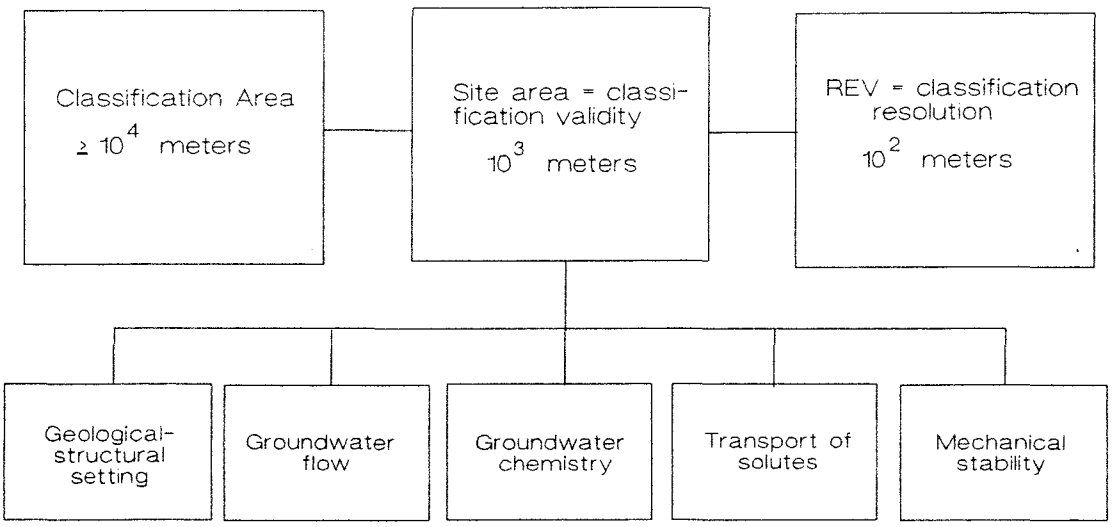

Figure 4.3. Schematic description of the scales and issues of the suggested strategy for geoscientific classifications.

4.3 GEOLOGICAL-STRUCTURAL SETTING

The overall purpose of the siting process is to identify areas where the possibilities for radionuclides to reach the biosphere, if the repository fails, are as small as possible. The repository site should therefore be selected away from major fracture zones, since they are regarded to be highly conductive to contaminant transport. Further, the repository should be located to an area of low rock type variability to facilitate repository construction. An assessment of the geological-structural setting thus forms a basis for characterization of the conditions for repository establishment and safety. There may be several ways to perform such an assessment. In the preinvestigations for the Äspö HRL, the following parameters were used to characterize the geological-structural setting (Gustafson et al, 1991):

* Major fracture zones
* Distribution of rock types (%)
* Rock boundary frequency (nos/100 m)

4.3.1 Major fracture zones

To be able to construct a repository with a high degree of safety, it has to be sited in a volume of rock free from major fault and fracture zones. There are a number of methods available for identification of major fault and fracture zones. Digital terrain models and satellite imagery have been used to good advantage for interpretation of this type of lineaments in Sweden, see e.g. Tirén et al (1987), Tirén and Beckholmen (1989), Gråsjö and Vestergren (1988), Gråsjö (1990), and Wladis (1992). There are several other methods for studying fracture and fault zones on large scales, e.g. geophysical methods and analyses of topographic maps. In several areas of Sweden the Geological Survey has produced tectonic maps in 1:50 000 scale.

An example of lineaments in crystalline rocks interpreted from digital terrain data is shown in figure 4.4.

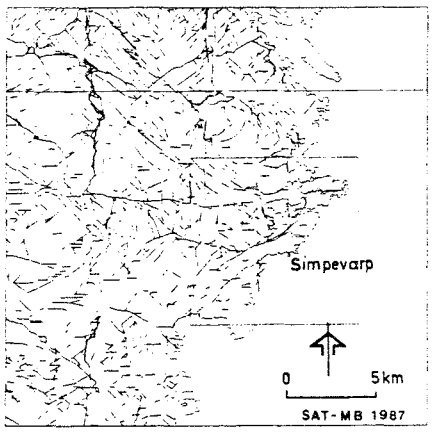

Figure 4.4. Lineament directions in the Simpevarp vicinity (from Tirén and Beckholmen, 1989).

Thus, there are workable techniques for identifying large scale fracture zones from existing information. This parameter is so important to the site selection process, that it has an overriding effect on other factors; no major fracture zones can be present in the rock volume occupied by the repository. A proper way to handle this parameter in the geoscientific classifications may be to accept only areas of repository size, which are free from major zones, for further classifications involving other critical parameters. All other areas should be discriminated.

Conclusion: It is suggested that the major fracture zones is included as a critical parameter for the geoscientific classification. This parameter is of primary importance for the safety and repository construction. It may be an overriding parameter so that all areas of repository size including major fracture zones, should be excluded from further classifications. Information about major fracture zones can be obtained from topographic maps, tectonic maps, digital terrain models, satellite imageries, etc.

Relevant prior estimates: Tectonic maps, topographic maps and lineament interpretations from digital terrain models and satellite imagery should be used to perform prior estimations regarding major fault and fracture zones.

4.3.2 Rock type distribution

The distribution of rock types is important to assess the building conditions for a repository. If there are many different rock types per unit area, the probabilities for making accurate predictions of the rock type at repository depths are small. In general terms, the rock type on the ground surface should probably have an extension of several km^2 to make it possible to find a repository sized block of the same rock type with a 50% accuracy. The rock type distribution is therefore suggested as a critical parameter for the geoscientific classification. The rock type distribution will primarily be estimated from geological maps.

Conclusion: The rock types distribution is suggested to be included as a critical parameter for the geoscientific classification. It is of primary importance for repository construction.

Relevant prior estimates: The rock type distribution can be estimated from geological maps.

4.3.3 Rock boundary frequency

The frequency of rock boundaries is, together with the rock type distribution, an important parameter to assess the building conditions for a repository. A small number of rock boundaries and rock types are advantageous for a repository construction. The rock boundary frequency is therefore suggested as a critical parameter.

Conclusions: It is suggested that the rock boundary frequency is included as a critical parameter for geoscientific classification. This parameter is of great importance for repository construction.

Relevant prior estimates: the rock boundary frequency can be estimated from geological maps.

4.4.4 Discussion

Some additional thoughts regarding the three suggested parameters can be expressed. It may generally be assumed that the major fracture zones and rock types observed at the ground surface can be traced down to repository depths. No studies have, however, been able to clearly confirm such assumptions. It should be remembered that due to erosional forces, the ground surface exposed today is only one of many possible horizontal sections of an initially much larger rock volume (figure 4.5). It can be argued that the section exposed today has a totally random vertical position. It may thus be expected that the distribution of lithological units and fracture zones at the surface in a statistical sense is a measure of the distributions at repository depths. Further research is needed to better understand how features displayed at the ground surface can be transformed to repository depths, and with what accuracy.

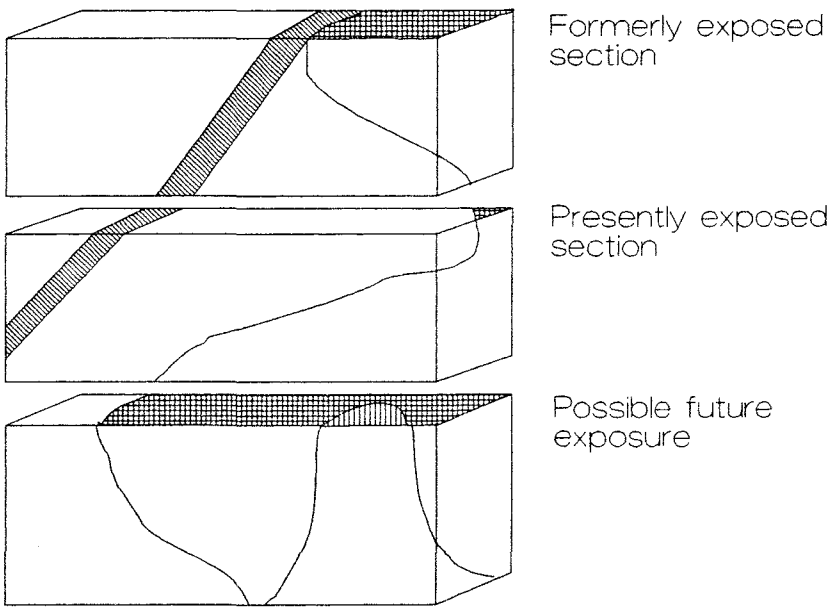

Figure 4.5. A conceptual outline of the presently exposed section of the bedrock in relation to earlier and future exposures.

The general lineament pattern representing faults and fracture zones on the Scandinavian peninsula may, e.g. according to Ronge (1988), be interpreted to have a rombic character. Ronge explained this pattern by the horizontal stresses resulting

from plate tectonic movements and the vertical stresses resulting from pressure release due to surface erosion. He also described the magnitude of the rombs to be in the order of 10^3 meters. A conceptual outline of the development of this rombic pattern is shown in figure 4.6.

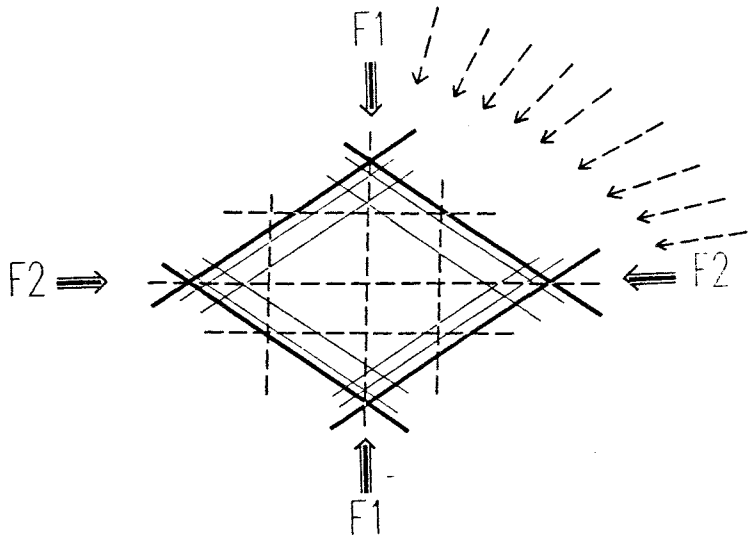

Figure 4.6. Outline of the development of rombic structures on the horizontal plane (Gråsjö and Vestergren, 1988 after Ronge, 1987).

During the preinvestigations at Äspö some fracture zones could be assumed taking this model into account. However, because of limited data giving difficulties to adequately match this model, these fractures could be assumed only with a very low degree of certainty. This model has been criticized by some workers stating that conditions are more complicated than this model can account for. Tirén (1991) presented a model of the geological setting and deformation history of a fracture zone and adjacent rock blocks at Finnsjön in Sweden. This work shows a far more complex structure of the geologic setting than does the rombic model suggested by Ronge.

There are several different opinions for how to interpret large scale fracture zones but for classification purposes it is important that the used model is applicable from an engineering geological point of view. This means that the model has to be adequately matched with respect to measured data and be useful for reasonable predictions rather than being absolutely true.

Further research is needed to get more accurate statistical background to make relevant predictions of the geological-structural setting. Existing models should be reviewed and reasonably accurate models developed for such predictions. Detailed investigation programs, as that at Äspö HRL and test sites, give good opportunities to perform such studies.

4.4 GROUND WATER FLOW

The groundwater flow is the amount of water per time unit that is transported through a cross-sectional area of the geological medium. It is the carrier for transport of any kind of contaminant through the subsurface. Groundwater flow conditions are determined by the geometry of pores and fractures of the geologic medium, the water density, the viscosity, the compressibility of water and fractures/pores, the gravitational field, and the pressure field. Groundwater flow on a large, or regional, scale in crystalline rocks is commonly described as a flow through a pseudo homogeneous porous media and with a flow direction governed by topographic conditions (figure 4.7).

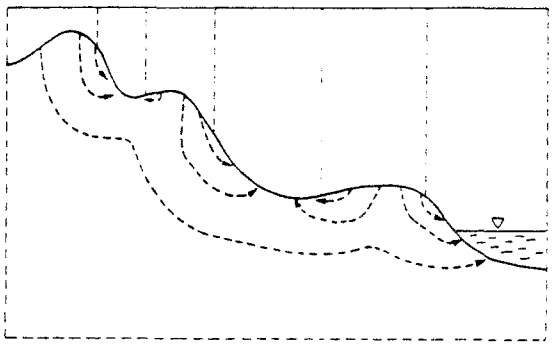

Figure 4.7. Large scale groundwater flow (from Svensson, 1984).

In more detail, however, there are large uncertainties regarding the flow conditions due to the great heterogeneities of fractured media. It has been concluded by several researchers, e.g. Moreno et al (1990) and Tsang and Tsang (1989) that flow and transport mainly take place along preferential flow paths or channels in fractured rocks. However, for classification purposes, it may be appropriate to study the groundwater flow on a regional scale, considering a REV-concept.

The specific ground water flow rate or flux is described by Darcy's law:

$$q = -\frac{dh}{dl}K \qquad (4.1)$$

where q = specific (Darcy) flux [m/s], - dh/dl = hydraulic gradient [d.l], and K = hydraulic conductivity [m/s].

For siting purposes a stochastic distribution for a critical Darcy flux $P(q_{cr})$ is wanted, so that $q_{cr} > q$ for all P. It is known that the groundwater flow rate has approximately a log-normal (SKI, 1991) or exponential distribution. The objective is then to estimate relevant expected values for hydraulic conductivity and gradient in order to calculate expected values on the groundwater flow rates. The strategy to estimate the expected values should be based on basic hydrogeological principles, and a possible approach is discussed below.

On a regional scale, hydraulic conductivity and hydraulic gradient locally have a negative correlation (figure 4.8).

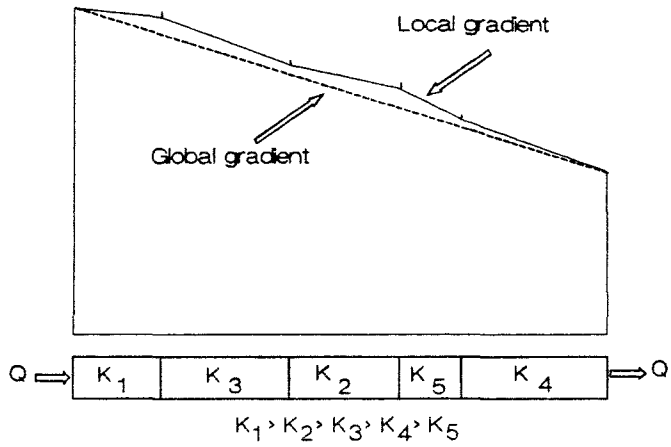

Figure 4.8. *The correlation between hydraulic gradient and hydraulic conductivity for one-dimensional groundwater flow.*

The correlation coefficient is defined as:

$$r(x,y) = \frac{E(xy)-E(x)E(y)}{\sqrt{\sigma_x^2\sigma_y^2}} \qquad (4.2)$$

where r = correlation coefficient, E = expected values of parameters, and σ^2 = variances of parameters.

If $-dh/dl = i$, this means that:

$$E(Ki) = E(K)E(i) + r(Ki)\sqrt{\sigma^2(K)\sigma^2(i)} \qquad (4.3)$$

Thus, the expected value for the product is always smaller than the product of the expected values of negatively correlated parameters. Therefore, a conservative expected value for q can always be estimated if the expected values for K and i, are known since $r(Ki)<0$.

There is a good knowledge of conductivity distributions for different rocks and hydrogeologic conditions, e.g. from the Äspö area. If the rock volume of interest can be treated as a continuous media, and if the head at the upper boundary of the aquifer is known, the pressure potential at every point in the subsurface can be determined (Gustafsson, 1970). Every type of ground surface profile and associated groundwater table conditions can be described by a summation of periodic functions. An example of this is shown in figure 4.10 where the land surface and groundwater table of two ridges and two valleys are described by the summation of two cosine functions:

$$\varphi_{y=0} = \frac{a}{2}[\cos\frac{2\pi}{b}x + \cos\frac{6\pi}{b}x] \qquad (4.4)$$

where the elements of this expression are explained in figure 4.9.

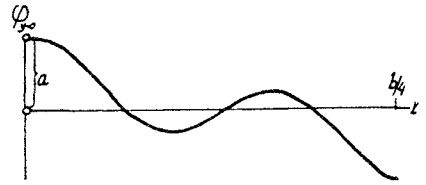

Figure 4.9. A setting of two ridges and valleys of land surface and groundwater table described by two added cosine functions (after Gustafsson, 1970).

From expression 4.4 Gustafsson (1970) calculated the equipotential lines and streamlines. The result is displayed in figure 4.10 showing recharge areas on ridges and discharge areas in the valleys. The surficial groundwater flow from the upper ridge is discharged in the upper valley, whereas the deeper groundwater flow from the upper ridge is transported to the lower valley.

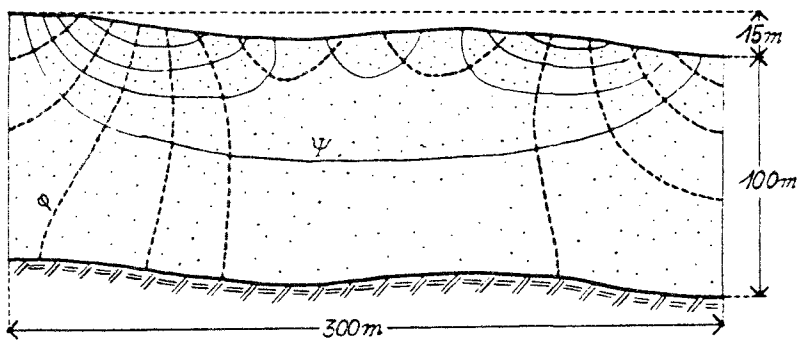

Figure 4.10. Streamlines and equipotential lines for the setting described in figure 4.10. φ and Ψ are equipotential lines and stream lines, respectively (from Gustafsson, 1970).

The given example above described two-dimensional flow along a profile, but the same approach is applicable also in three dimensions since the topographic conditions can be described as a Fourier series in three dimensions. However, to determine a hydraulic gradient distribution for a specific depth below ground surface in two dimensions is not very easily performed mathematically, especially when considering heterogeneities of the geologic medium.

The Darcy flux is the groundwater flux rate per cross sectional area of the rock. Since most of the cross sectional area is impervious and the ground- water flux only occurs in the pores and fractures, the porosity has to be accounted for to estimate the actual mean groundwater velocity. This velocity is defined as:

$$\bar{u} = \frac{q}{\theta} \qquad (4.5)$$

where $\bar{u}$ is the mean groundwater velocity and θ is the rock porosity.

The mean groundwater velocity is thus always higher than the Darcy velocity. The groundwater velocity is only of interest for non-sorbing nuclides since the porosity does not significantly influence the transport velocity of the sorbing species (Neretnieks, 1990).

Conclusion: it is suggested that hydraulic conductivity and hydraulic gradient are included as critical parameters for the geoscientific classification.

> **Relevant prior estimations:** conductivity distributions for different rocks from a large number of existing data and calculations of the hydraulic gradient distribution from topographic conditions should be used for calculating expected values of groundwater flow rates.

4.5 TRANSPORT OF SOLUTES

There are four main processes that are frequently discussed in the literature as being important for solute transport:

* Groundwater flow
* Dispersion
* Diffusion
* Sorption

The transport and sorption processes in a fracture are schematically displayed in figure 4.11.

The groundwater flow has been discussed in the previous section and emphasis is therefore put on the three other processes here. Although these processes are regarded as being important to describe the transport of radionuclides in fractured media, there are some uncertainties and disagreements regarding specific processes, e.g. the importance of matrix diffusion. It is beyond the scope of this study to verify the specific processes, and emphasis is put on handling of parameters that may be critical for the transport conditions. The suggested classification strategy is flexible and if future research shows that some process is missing or irrelevant, the list of critical parameters can, and should be, revised.

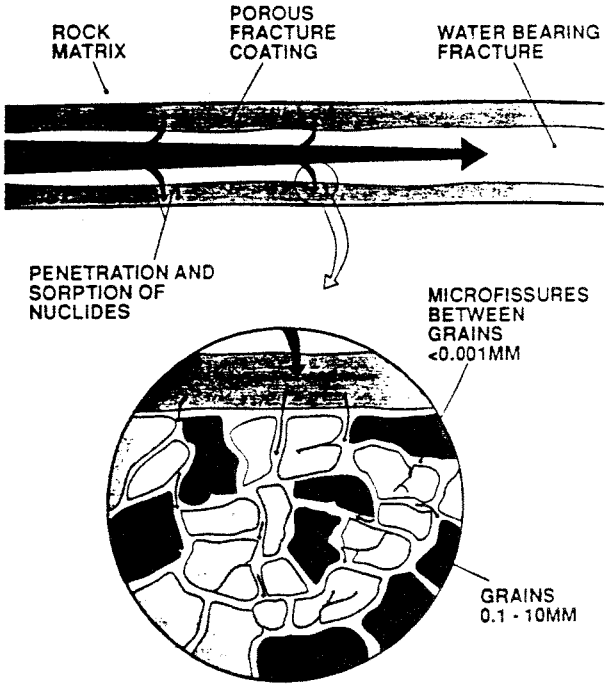

Figure 4.11. Transport and sorption processes in a fracture (from SKI, 1991).

4.5.1 Dispersion

Dispersion occur in fractured media through the parabolic profiles of the velocities inside a fracture, through different degrees of aperture between fractures, and by mixing when fractures of different directions intersect (de Marsily, 1986). There are different opinions regarding the effects of dispersion. A large dispersion may dilute a contaminant plume, which would therefore arrive to the geosphere at a lowered concentration. On the other hand, for radionuclide transport this may not necessarily be true, since radionuclides decay. Instead, the residence time of the contaminant may be important, so that although one portion of a contaminant plume is diluted through dispersion it may have a considerably higher activity than another portion of the plume which travels with a longer residence time (Neretnieks, 1990).

The dispersion depends on the degree of mixing between streamlines. In the "classical" concept of advective-dispersive transport it is assumed that the mixing between streamlines is so large that the dispersion coefficient, D, can be regarded as being proportional to the average groundwater velocity and that the dispersion length, or dispersivity, is constant:

$$D = \alpha \frac{q}{\theta} \qquad (4.6)$$

where D = dispersion coefficient [m^2/s], α = dispersivity constant [m], q = specific flux [m/s], and θ = rock porosity [d.l].

However, in crystalline rocks at large depths, fissures are far apart and long distances are therefore required for mixing. This means that the dispersivity cannot be regarded as constant unless migration distances are very long (Neretnieks, 1990). Neretnieks (1983) showed that as long as flow channels do not intersect, dispersivity is proportional to distance and never becomes constant. Because of the low frequency of fissures at large depths it is, according to Neretnieks (1990), not clear that the mixing capabilities are sufficient to let the dispersivity become constant and independent of distance before the contaminant reaches a fracture zone with different properties. It was suggested by de Marsily (1986) that the dispersion equation is only valid after large times or large migration distances, up to 10 times the characteristic length of the geological structures of the medium.

Several investigations (Landström et al, 1978; Webster et al, 1970; Geldhar, 1987) show that dispersivity tends to increase with migration distance (figure 4.12).

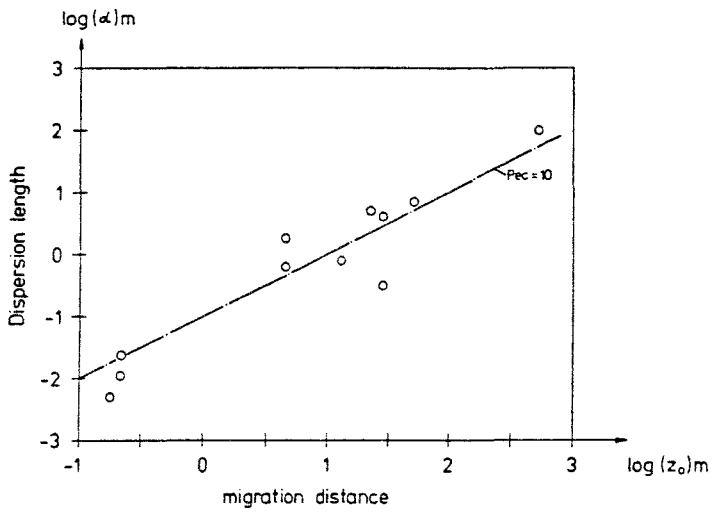

Figure 4.12. Dispersion in fractured rock as a function of migration distance (from Neretnieks, 1990).

It has further been shown that the dispersivity is <u>not</u> an intrinsic property of the geologic medium, but depends also on the variability of the groundwater flow field (de Marsily, 1986; SKI, 1991). A high flow field variability indicates a stronger correlation between dispersivity and migration distance than does a low flow field variability.

To account for the migration distance and the flow field variability it may be appropriate to describe the dispersivity using the Peclet number. The Peclet number is a measure of the relationship between dispersion and advection and takes into account the groundwater velocity and the characteristic length, or the heterogeneities, of the geologic structure. Discrete network analyses suggest that the development of the Peclet number (or dispersivity) with migration distance is a key to determining the transport characteristics of fractured rock (SKI, 1991). The Peclet number is defined as:

$$Pe = \frac{Xq}{D\theta} = \frac{X}{\alpha} \qquad (4.7)$$

where Pe = Peclet number [d.l], X = a characteristic length (e.g. the migration distance) [m], see above for others.

Low Peclet numbers indicate that dispersion is high. Studies (SKI, 1991) show that flow in crystalline rocks at large depths are generally associated with low Peclet numbers (0-4) with a log-uniform distribution. Extremely high values are related to channeling effects. In general, large Darcy flux is associated with high Peclet numbers (SKI, 1991).

Discrete network analyses performed by Dverstorp and Andersson (1989) and Dverstorp (1991) showed that if the groundwater flow variability is low, the breakthrough from a discrete model can be well described using the "classical" advection-dispersion assumption (figure 4.13). This means that dispersion can be described with a constant dispersivity, i.e the Peclet number is proportional to the migration distance. For cases with a higher groundwater flow field variability the match between the discrete network model and the advection-dispersion assumption is in some cases poor (figure 4.14). In those cases, the dispersion cannot be described with a constant dispersivity and the Peclet number tends to be constant with travel distance (figure 4.15). As also seen in figure 4.16, some realizations give fairly high Peclet numbers (6-8), which indicates fast transport and low dispersion, i.e channeling. The probability of obtaining such channeling effects increases with increased groundwater flow variability (SKI, 1991).

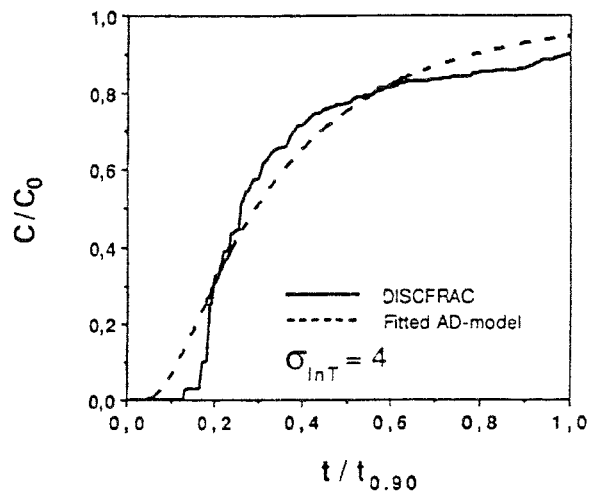

Figure 4.13. Normalized cumulative breakthrough curves from a discrete fracture network realization in a 20 meters long domain. Solid curves represent the discrete model and dashed curves represent a fitted advection-dispersion model (from Dverstorp, 1991).

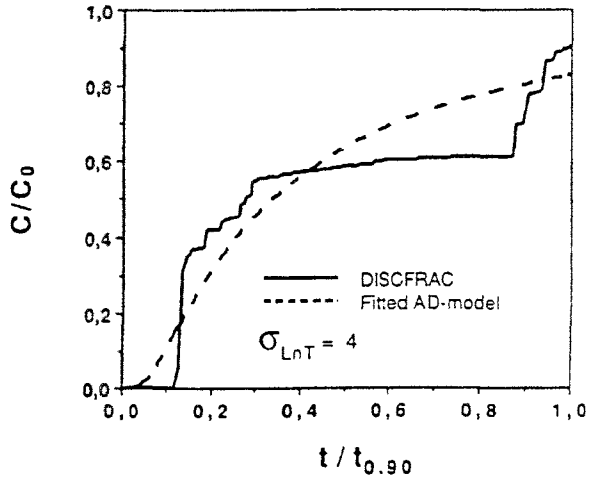

Figure 4.14. Normalized cumulative breakthrough curves from a discrete fracture network realization with pronounced channeling in a 20 meters long domain. Solid curves represent the discrete model and dashed curves represent a fitted advection-dispersion model (from Dverstorp, 1991).

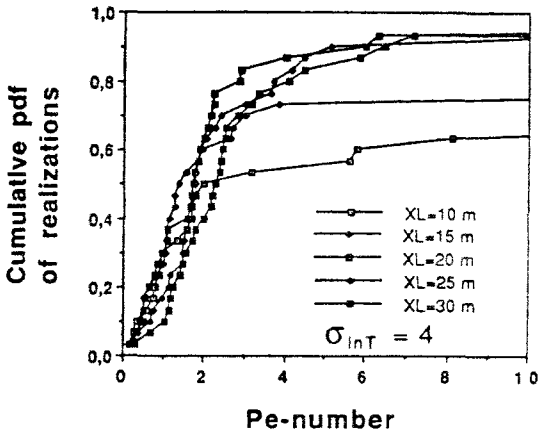

Figure 4.15. Cumulative frequency plot of estimated Peclet numbers in individual discrete fracture network realizations, for different migration distances, XL (from Dverstorp, 1991).

In addition to the groundwater flow variability, the connectivity of the rock is also an important parameter to determine the Peclet number (SKI, 1991). The connectivity depends on the fracture geometry, e.g fracture size, orientation, and density. It was shown by Dverstorp and Andersson (1989) that networks with similar connectivities but different combinations of fracture size, orientation, and density, have to a great extent similar properties. Dverstorp and Andersson (1989) described how to estimate the connectivity from field-observations in the Stripa mine.

Conclusions: The development of the Peclet number with transport distance is a key to determining the transport characteristics of fractured rock and should be included as a critical parameter for geoscientific classifications. The groundwater flow variability and the connectivity of the rock are the main factors that determine the Peclet number.

Relevant prior estimates: Based on existing knowledge, the Peclet number generally varies between 0 and 4 on large depths in crystalline rocks, unless channeling effects are present. SKI (1991) suggested within Project-90 that a log-uniform distribution should be used for probabilistic purposes.

4.5.2 Matrix diffusion and sorption

Diffusion occurs because of pressure and concentration gradients between pores or between fractures and pores. In the case of radionuclide transport in fractured media, the effect of diffusion from fractures to the pores of the rock matrix is of great interest. If matrix diffusion takes place, the possibilities for sorption are greatly increased since the rock matrix will provide a much larger specific surface than the fracture walls.

There are several studies indicating that taking only advection and dispersion into account give a poor transport model. Neretnieks (1990) suggested that matrix diffusion may in fact be a dominating driving force of nuclide transport, due to the long contact time between water and rock at large depths. Two safety analyses, KBS-3 (1983) and NAGRA (1985), indicated that matrix diffusion is by far the most important mechanism for retardation of radionuclides.

One way to describe the diffusion is through the formation factor for matrix diffusion:

$$F_f = \frac{\theta \delta_D}{\tau^2} \qquad (4.8)$$

where F_f is the formation factor [d.l], θ is the transport porosity [d.l], δ_D is the constrictivity of the pores [d.l], and τ is the tortuosity of the pores [d.l]

If all solutes were influenced in the same way by the pore system, then it would suffice to measure the formation factor for one solute. This is not always the case, but F_f can still be a valuable entity for comparison purposes (Neretnieks, 1990). Skagius and Neretnieks (1986a) determined the effective diffusivities and formation factors for different rock materials and nonsorbing species, e.g iodide. They showed that the diffusivity and the formation factor vary to a great extent between gneiss and granite taken from the same drillcore. They also showed that the total diffusivity in rock plus fracture filling minerals is of the same order of magnitude or higher than in rock without fracture coating materials. This means that the diffusivity or formation factor of the parent rock material can be used as a conservative estimate of the diffusion capacity.

Skagius and Neretnieks (1986b) showed that the formation factor values determined in diffusion experiments are in fair agreement with those determined from electrical resistivity measurements for the same rock materials. The relationship between the formation factor, the resistivity and the effective diffusivity is (Skagius and Neretnieks, 1986b):

$$\frac{D_e}{D_v} = F_f = \frac{R_0}{R_s} \qquad (4.9)$$

where D_e is the effective diffusivity [m^2/s], D_v is the bulk phase diffusivity of the diffusing component [m^2/s], R_0 is the is the resistivity of the water contained in the rock [Ωm], R_s is the resistivity of the saturated rock sample [Ωm], and F_f is the formation factor [d.l].

The advantage of using resistivity and the formation factor as a measure of the diffusion is that resistivity measurements are more easily and quicker performed than diffusion experiments.

Conclusions: For geoscientific classification it is suggested that the formation factor for different rock materials is included as a critical parameter.

> **Relevant prior estimates:** existing results from formation factor measurements on different rock types should be used as prior estimates. Resistivity measurements can give reasonable values on the formation factor.

4.5.3 Fracture surface sorption

In the previous section matrix diffusion was discussed. Those elements affected by matrix diffusion can be regarded as sorbed and permanently extracted from the fracture flow system. For nuclides still in the fracture flow there is an opportunity for sorption onto the fracture surfaces. The uncertainties regarding this parameter are large and the sorption mechanisms for fractured media are not well understood. It is, however, due to its importance for contaminant transport suggested that the possibilities for describing fracture sorption in the geoscientific classification are explored.

Sorption is a term describing several processes. It is common to divide the sorption processes as follows (SKI, 1991):

1. Physical adsorption caused by van der Waal type forces.

2. Electrostatic adsorption, which is in principal equal to ion exchange, and is due to the same kind of coulomb forces as acting between ions in solution.

3. Chemical substitution can occur if ions in the solution are able to take the place of similar elements in the solid mineral structure.

4. Chemisorption which cover all kinds of interactions except those belonging to physical and electrostatic adsorption. Chemisorption would mainly involve interactions with contributions from covalent bonding.

Most safety assessments have until now used the so-called K_d-concept for sorption characterization. This approach make use of constant distribution coefficients, K_d:s, or retardation factors, R:s. The K_d-concept has been criticized by several researchers, but according to SKI (1991) it is still valuable for practical purposes, and will be also in the foreseeable future, because of its simplicity.

The distribution coefficient is generally defined as:

$$K_d = \frac{\textit{mass of solute on the solid phase per unit mass of solid phase}}{\textit{concentration of solute in solution}}$$

given the dimension [m^3/kg].

Table 4.1 shows K_d:s representative for normal groundwater in contact with fracture fillings of calcite mixed with some iron hydroxide in granitic rocks. Table 4.1 also shows the great differences of the K_d for different chemical environments. The chemical environment need therefore to be described with respect to well-defined values on parameters such as pH and Eh. The "poor chemistry" values of table 4.1 were thought to result from a lower abundance than expected of sorbing minerals, an unfavorable aqueous chemistry with e.g. organic complexing and high salinity, or a combination of both these factors.

Table 4.1 shows K_d with respect both to oxidizing and reducing conditions. Typically the chemical conditions of groundwater at repository depths are reducing. This data was compiled by Andersson (1991) for the Project-90 sorption database.

The K_d concept assumes reversible sorption and instantaneous attainment of equilibrium. Such conditions are almost never fully achieved in natural systems. However, these assumptions will in most cases lead to an overestimate of the migration rates in transport calculations. (SKI, 1991).

For contaminant migration through fractured media when only sorption on the fracture surfaces is of interest, the distribution coefficient should be altered and expressed with respect to the specific surface area of the fractures rather than the density of the geologic media (Burkholder, 1976):

$$Ka = \frac{\textit{mass of solute on the solid phase per unit area of solid phase}}{\textit{concentration of solute in solution}}$$

Table 4.1. Sorption distribution coefficients in granite for different nuclides (SKI, 1991).

Element	Oxidizing conditions		Reducing conditions	
	Best estimate [m3/kg]	Poor chemistry [m3/kg]	Best estimate [m3/kg]	Poor chemistry [m3/kg]
Am	5.0	0.5	5.0	0.5
Pu	3.0	1.0	5.0	0.5
Np	0.01	0.001	5.0	0.1
U	0.01	0.002	5.0	0.01
Pa	0.1	0.01	0.1	0.01
Th	5.0	0.01	5.0	0.01
Ra1)	0.1	0.005	0.1	0.005
Cs	0.05	0.005	0.05	0.005
I	0	0	0	0
Sn2)	0.01	0.001	0.01	0.001
Tc	0.0002	0	0.005	0
Zr	4.0	0.1	4.0	0.1
Sr	0.004	0.001	0.004	0.001
Se2)	0.001	0.001	0.001	0.001
C2)	0.05	0.005	0.05	0.005

1) The poor chemistry values for Ra were by implication 0.0002, since the same fixed ratio between Ra and Th data was used as for the best estimate.

2) See Worgan and Robinson (1991).

A retardation factor for contaminant transport through fractured media can then be expressed as (Freeze and Cherry, 1979):

$$R = \frac{\bar{u}}{\bar{u}_c} = 1 + AK_a \qquad (4.10)$$

where R = the retardation factor for fracture surfaces [d.l], $\bar{u}$ = the average linear velocity of the groundwater, $\bar{u}c$ = is the velocity of the C/C0 = 0.5 point on the concentration profile of the retarded constituent, Ka = the surface sorption distribution coefficient [m], and A = specific surface of the fracture [m2/m3].

Also here the chemical environment needs to be characterized to make the assessments of the distribution coefficient and retardation factor valuable. It can thus be concluded that the sorption distribution coefficient is associated with great uncertainties, whatever the form of expression. A use of Kd:s or Ka:s for classification purposes is therefore not considered to be realistic.

As an alternative to the distribution coefficients, the specific surface area may be of interest. The specific surface area exposed to the contaminant is, as shown in expression 4.10, of great importance to the retardation capabilities of the contaminant and may be a fair enough measure of the sorptive capacity of the fractures. This area is, however, in most cases not equal to the total specific fracture surface area of the rock volume, since contaminant transport will not occur in all fractures, but will be restricted to preferential paths (Tsang and Tsang, 1989; Moreno et al, 1990). The effective specific surface will thus be smaller than the total specific surface. Using a log standard deviation of fracture transmissivity for stochastic realizations, it was found that the effective specific surface may in general be less than 10% of the total specific surface area (SKI, 1991).

A pessimistic value of the effective specific surface was estimated within the SKI Project-90 (SKI, 1991) to be 10^{-2} m^{-1}. The possibilities for estimating this surface area for different rock types need, however, to be further explored. SKI (1991) thus pointed out that much more work can and should be done to increase the knowledge of the effective specific surface area. It was suggested that first of all, field experiments should be performed specifically to measure the effective specific surface.

Conclusions: It is suggested that it is attempted to include the effective specific surface as a critical parameter in the geoscientific classification process. More studies are however needed to evaluate how to optimally assess this parameter.

Relevant prior estimates: Estimates of the total specific surface is very uncertain due to lack of knowledge. The estimates presented by SKI (1991), in the order of 10^{-2} m^{-1}, may at present be the most realistic one.

4.6 MECHANICAL STABILITY

The mechanical stability are of importance for the ability of the rocks to withstand future changes of stress and for the building conditions at the repository. Future changes of stresses, will primarily be due isostatic and eustatic effects from glaciations. Glaciations are regarded to be more important than plate tectonics during he time span of interest. Glacials and stadials stress the earth crust and may, although not likely (SKI, 1991), give reopening of fractures as well as altered hydrologic conditions within the bedrock, e.g changed flow directions. In general, southern Sweden may be less vulnerable than the northern parts since ice caps will be thinner and have a shorter duration in the south than in the north. Factors having an impact on the stability of the bedrock may be:

* Ice cap presence
* Glaciation duration
* Permafrost depth and duration
* Number of glacials and stadials
* Number, duration and magnitudes of eustatic changes

Several studies of the effects of large ice loads on a repository have been performed, e.g. by Shen and Stephansson (1990). Attempts have also been made to model future glaciations in Scandinavia. The analysis performed by Shen and Stephanson implied that for the Reference Site within Project-90 (SKI, 1991), most stress changes are relieved through small movements in major fault zones leaving the repository principally unaffected.

The mechanical stability is regarded to be of primary importance for the geoscientific classification also with respect to the building conditions of the rock and the safety of the repository. The stability of the rock block selected for the repository has to be very good in order to a construct a repository that fulfills the requirements during the time span considered.

To assess the mechanical stability of the rock mass, some kind of rock classification is generally performed. The RMR index by Bieniawski (1979) is a common classification methodology used for predictions of the mechanical stability. The system is less descriminating than some other systems, e.g. the Barton Q-value (Barton et al, 1974), and is thus less sensitive to misjudgments and poor data. It still gives results that are precise enough for most underground constructions in rocks (Bäckblom et al, 1984).

The RMR factor is:

$$RQD + IRS + JS + JC + GW = RMR \qquad (4.11)$$

where RQD = Rock Quality Designation or Deere's drill core quality rating, IRS = strength of intact rock material (point load strength or uniaxial compressive strength), JS = joint spacing, JC = condition of joints, and GW = ground water conditions.

The RMR index is a value between 1 and 100 divided into the following classes:

< 20	very poor rock
21-40	poor rock
41-60	fair rock
61-80	good rock
81-100	very good rock

Table 4.2 shows an outline of the RMR system.

Table 4.2. Rock Mass Rating System (RMR).

A. CLASSIFICATION PARAMETERS AND THEIR RATINGS

	Parameter		Ranges of Values						
1	Strength of intact rock material	Point-load strength index (MPa)	>10	4-10	2-4	1-2	For this low range, uniaxial compressive test is preferred		
		Uniaxial compressive strength (MPa)	>250	100-250	50-100	25-50	5-25	1-5	<1
	Rating		15	12	7	4	2	1	0
2	Drill core quality RQD (%)		90-100	75-90	50-75	25-50	<25		
	Rating		20	17	13	8	3		
3	Spacing of discontinuities		>2 m	0.6-2 m	200-600 mm	60-200 mm	<60 mm		
	Rating		20	15	10	8	5		
4	Condition of discontinuities		Very rough surfaces Not continuous No separation Unweathered wall rock	Slightly rough surfaces Separation < 1 mm Slightly weathered walls	Slightly rough surfaces Separation < 1 mm Highly weathered wall	Slickensided surfaces or Gouge < 5 mm thick or Separation 1-5 mm Continuous	Soft gouge > 5 mm thick or Separation > 5 mm Continuous		
	Rating		30	25	20	10	0		
5	Groundwater	Inflow per 10 m tunnel length (L/min)	None	<10	10-25	25-125	>125		
		or	or	or	or	or	or		
		Ratio $\frac{\text{Joint water pressure}}{\text{Major principal stress}}$	0	<0.1	0.1-0.2	0.2-0.5	>0.5		
		or	or	or	or	or	or		
		General conditions	Completely dry	Damp	Wet	Dripping	Flowing		
	Rating		15	10	7	4	0		

The RMR method is a qualitative guideline method (like DRASTIC) for different kinds of construction work in rocks. It does not give answers in real, quantitative parameter values but has proven to be very useful for building purposes. The RMR index is regarded to be the most useful estimation technique available for stability assessments for the geoscientific classification.

Since the RMR index has been widely used, there are data and knowledge available to perform good prior estimations. RMR assessments are common practice for a variety of building purposes in rocks, e.g. tunnel excavations. Bieniawski (1989) presented RMR estimations from 351 case histories. The RMR index was used and estimated by Stille (Gustafson et al, 1991) in the preinvestigations at Äspö as a measure of the building conditions of the HRL.

Conclusions: It is suggested that the RMR index is included as a critical parameter for the geoscientific classifications with respect both to the ability to withstand future changes in stress of the rock mass and the building conditions of the rock mass.

Relevant prior estimates: There is an abundance of RMR assessments fROM various construction projects and there exist good knowledge for performing prior estimates of this parameter. Gustafson et al (1991) performed estimations, based on professional judgments, of RMR distributions for different rock blocks at Äspö HRL prior to excavation. These estimations showed an average distribution for the four rock blocks as follows:

RMR	Average %
> 72	31
60-72	40
40-60	21
> 40	8

4.7 GROUNDWATER CHEMISTRY

The groundwater chemistry is of importance for several factors that may affect present and future transport conditions at repository depth, e.g weathering and precipitation in fractures. The Swedish deep groundwater chemistry is generally well known with regard to pH, Eh, the most common ions and their concentrations (SKI, 1991). Typically, the chemical environment is reducing in deep groundwaters.

The chemical conditions of groundwater in the Swedish crystalline bedrock have been stable for a long time, indicated by saline waters of high ages found at repository depths. The waters found at Äspö (figure 4.16) show an increasing salinity with depth and is at repository depth several thousand years old. The most likely explanation to these observations is that the groundwater originated from sea water from the Litorina stage of the Baltic Sea, 7000 to 3000 B.P., after which Äspö rose above sea level. Also at other sites, more inland, saline waters are found at large depths.

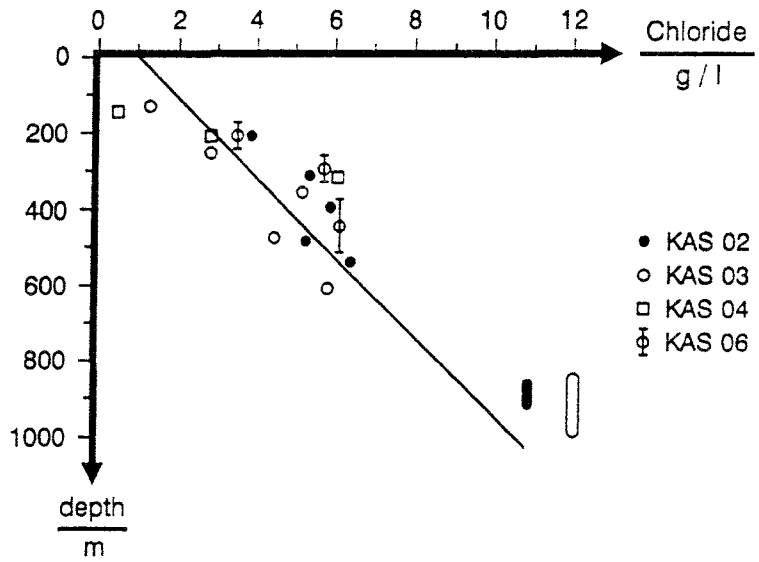

Figure 4.16. The chloride concentration as a function of depth in boreholes KAS02, 03, 04, and 06 at Äspö (from Wikberg et al, 1991).

Characterization of the groundwater chemistry at repository depths requires several parameters. In the preinvestigations for the Äspö HRL ion content, Eh, pH, and salinity were used to describe the groundwater chemistry. These parameters may be of interest also for classification purposes. There are two issues of groundwater chemistry that may be of primary importance for repository siting:

1. Whether the environment is reducing or oxidizing is of importance for sorption possibilities.

2. The salinity of the groundwater. Saline water may cause a barrier for nuclide transport from the repository through the geosphere.

Modern methods of in situ measurements of pH and Eh clearly show that deep groundwaters are reducing, with low Eh values, usually between -200 and -350 mV (SKI, 1991). This was shown also from measurements at Äspö (Wikberg et al, 1991).

Wikberg et al (1991) argue that Eh is primarily controlled by the concentration of dissolved ferrous iron and ferric oxy-hydroxide in an environment with low oxygen content, such as in deep groundwaters. Since Eh is closely related to iron content, it may be appropriate to use the relation of Fe^{2+}/Fe_{tot} (total iron content) to assess the redox-potential. Even if the redox conditions do not change very much between different areas, this parameter is of primary importance to describe the repository conditions and should be included in the classification process. The iron content depend primarily on the mineralogy composition of the geological media and it may be advantageous to use this parameter instead of Eh directly, since it is a more straightforward process to evaluate the iron relation rather than Eh from existing data, such as geological maps. According to Wikberg et al (1991, table 3.24) the sampled groundwaters at Äspö showed a relation between 0.86 and 1. This parameter has this an advantageous character for classification purposes (varies between 0 and 1) and a conservative estimation of this parameter should be possible to perform before any measurements are taken.

Salinity is also regarded to be a very important parameter for classification purposes. A high salinity is advantageous since it gives a stable density stratification which decreases the possibilities for groundwater to reach the biosphere through heat convection from the repository. Saline groundwater may thus cause a natural barrier between the repository and the biosphere. The salinity should be possible to estimate from knowledge of the geologic history, distance from present and past coastlines, and existing data from mines and SKB test sites.

Conclusions: It is suggested that salinity and the Fe^{2+}/Fe_{tot} relation are included as critical parameters for the geoscientific classification.

Relevant prior estimates: The salinity can be estimated to an acceptable degree of confidence from existing knowledge and data, e.g. from mines and SKB test sites. Since the conditions at repository depths generally are reducing

and existing information show a value close to 1 for the Fe^{2+}/Fe_{tot} relation, it should be possible make conservative estimations of this parameter. According to the Äspö investigations the Fe^{2+}/Fe_{tot} relation generally varies between 0.86 and 1.

4.8 DISCUSSION

In this chapter a set of 11 parameters have been suggested for inclusion into the geoscientific classification methodology:

* Major fracture zones
* Rock type distribution
* Hydraulic gradient
* Formation factor (matrix)
* RMR
* Salinity
* Rock boundary frequency
* Hydraulic conductivity
* Peclet number
* Effective specific surface
* Fe^{2+}/Fe_{tot} relation

All parameters may not be easily assessed from today's knowledge and data. Further research is therefore needed to fully evaluate how to optimally assess these parameters. Also, the set of parameters is not regarded to be definite, but is a suggestion based on a literature review and regarded as being of interest with respect to the classification strategy described in chapter 3.

The parameters have been suggested primarily with respect to their importance to the construction and performance of the repository and not for a complete description of the geoscientific environment. The classification process suggested here has thus a practical, engineering geological approach. Therefore, all parameters may not vary very much between different areas prior to detailed studies, e.g. the Fe^{2+}/Fe_{tot} relation, but have been included in order make the classification results describe the conditions for repository construction in relevant terms.

It is suggested that the set of parameters is thoroughly reviewed and revised if necessary. It is the opinion of the authors that the set of parameters should be established through consensus within the geoscientific society. The set of parameters presented here should thus be regarded as a starting point for the parameter selection process.

5 AN EXAMPLE OF BAYESIAN UPDATING

5.1 INTRODUCTION

In classifications of a large areas the evaluator is primarily directed to limited data and professional knowledge from past experiences. The first, or prior, estimate of a parameter has in many cases to be based on professional judgments before any measurements are taken. Given the classification approach described in chapter 3, prior estimates should be updated as new data become available. To perform this updating in the geoscientific classification process a Bayesian approach was suggested in chapter 3.

The objective of this section was to show how to perform an updating of a prior estimate using Bayesian statistics. RQD (Rock Quality Designation) was regarded as being a suitable parameter for this purpose. RQD-measurements have been performed on drill cores from Äspö and this parameter does not require that a conceptual model is accepted before any discussions regarding its implications can be performed.

In this section prior estimates of RQD, based on professional judgments only, are successively updated using measurements from drill cores. In the updating process, the sequence of drilling campaigns in the area was followed in order to carry out a most realistic example. The updatings were performed in three steps, using measurements from three areas, or rock blocks, investigated during the siting of the Äspö HRL.

5.2 BLOCK DESCRIPTIONS

The volume of the rock block influenced by the first drillings, KAS02, KAS03, and KAS04, was in this example designated to be 750 m long, 500 m deep, and 100 m wide, and is a section connecting the three drillings. This block is referred to as the test block.

The access tunnel lies within a block that has a length of 775 meters, a depth of 200 meters below ground surface, and a width of 50 meters. This is referred to as the access tunnel block. With the exception of the block width, this corresponds to the dimensions for the access tunnel block used in the preinvestigations at Äspö.

The target volume for the HRL is situated 200 meters below ground surface. In this example the dimensions of this block is a cylinder with a radius of 200 meters and a height of 300 meters. The actual volume is somewhat larger but for simplicity reasons the volume has been restricted to given dimensions. This block is referred to a the target block.

For a more detailed description of the different blocks the reader is directed to Gustafson et al (1991). The locations of the blocks and drillings are shown in figure 5.1.

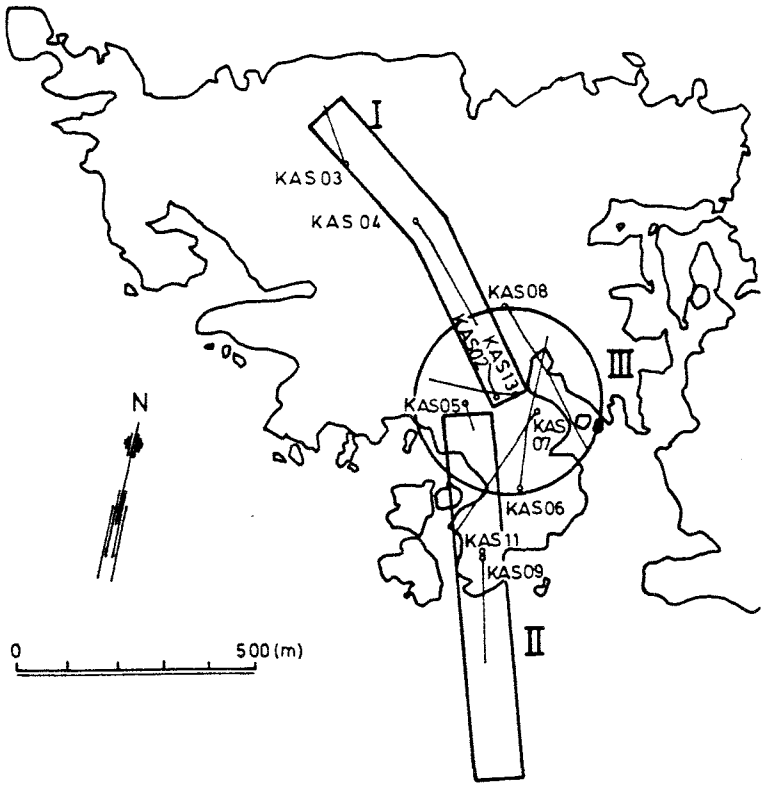

Figure 5.1. The locations of the test block (I), the access tunnel block (II), the target block (III), and the drilling locations at Äspö.

5.3 PRIOR ESTIMATES

Before the measurements from Äspö were studied, a prior estimate of the RQD was made based on professional judgments. There are few published studies on RQD distributions for different rock types and structural settings. However, within the preinvestigations for the Äspö HRL, predictions of the RMR-index were carried out by Gustafson et al (1991). Assuming that RQD varies in a similar way compared to the RMR, a prior estimate of the RQD distribution can be simulated for the Äspö area before considering any measurements.

The distribution of table 5.1. was considered to be a relevant measure of an RQD distribution for good quality crystalline rocks. It was therefore used as a prior distribution in the updating process using the boreholes in the test block, i.e. KAS02, KAS03, and KAS04.

Table 5.1. Prior RQD-distribution for updating of the test block.

RQD	Class	%
0-25	1	5
25-50	2	10
50-75	3	20
75-100	4	65

5.4 UPDATING FUNCTION

The following expression is in a Bayesian context. The RQD-distribution of the volume influenced by each measurement, i.e drilling, is assumed to be known with certainty after the drilling has been performed. The prior estimates is modified after each drilling with respect to the volume influenced by the drilling, so that:

$$P_P(RQD) = P_M(RQD)\,V_M + P_A(RQD)\,(1-V_M) \qquad (3.1)$$

where P_P is the posterior probability, P_M is the measured probability, P_A is the prior probability, and V_M is the percentage of the entire block volume influenced by the measurements.

The prior distributions were updated using measurements from one drilling at a time. The posterior probability from the first updating is used as a prior probability of the second updating, and so on.

5.5 UPDATING ASSUMPTIONS

For the updating it was assumed that the volume influence by the drillings were 50 meters from the drill core, i.e. the RQD values observed at the drill core can be autocorrelated 50 meters into the rock mass. No studies have been found that have aimed at assessing the autocorrelation of a drilling with respect to RQD. It is, however very important to have such knowledge in performing the updating process since the autocorrelation has a large significance on the results. 50 meters was, based on professional judgments, regarded to be a relevant value.

Assuming the radius of influence to be 50 meters, a volume of 7854 m^3 is influenced by every meter that is drilled. From this value, the percentage of influenced rock volume of the access tunnel block and the target area, respectively, can be calculated and used as V_M in the updating function. For example, drilling KAS05 penetrates the target block for 300 meters. The volume of the target block is:

$$200^2 * \pi * 300 = 3.8 * 10^7 \text{ m}^3$$

The percentage of the entire target block that is influenced by drilling KAS05 is then:

$$7854 * 300/3.8 * 10^7 = 6.2\%$$

The influences of all boreholes were calculated this way.

5.6 RESULTS

The updating procedure was carried out in three steps as explained above, starting with updating of the test block. The posterior estimates from this block were used as prior estimates for the updatings of the access tunnel block and the target block. The distributions from the RQD measurements for the borehole sections that were used for the updating procedure is shown in table 5.2.

Table 5.2. *Frequency distributions for the RQD measurement used for the Bayesian updating process.*

	%RQD=1	%RQD=2	%RQD=3	%RQD=4
KAS02	5.8	0	16.7	77.5
KAS03	1	11.8	14	73.2
KAS04	8.8	3.4	19	68.8
KAS05	0.9	5	5.3	88.8
KAS06	0.7	6.5	8.8	84
KAS07	4.7	11.2	3	81.1
KAS08	0.3	0	6.3	93.4
KAS13	10.9	0.7	9.2	79.2
KBH02	16.4	1.2	12.8	69.6
KAS09	14.1	2	7.4	76.5
KAS11	14.4	2.2	7.3	76.1

5.6.1 Test block

The three drillings KAS02, KAS03, and KAS04 were used for updating in this block. The updatings were performed as shown below:

<u>KAS02</u>: $P_{P1}(RQD > 75\%) = 0.775 * 0.104 + 0.650 * (1-0.104) = 0.663$

<u>KAS03</u>: $P_{P2}(RQD > 75\%) = 0.732 * 0.104 + 0.663 * (1-0.104) = 0.670$

<u>KAS04</u>: $P_{P3}(RQD > 75\%) = 0.688 * 0.100 + 0.670 * (1-0.100) = 0.672$

It can be shown that final result is the same regardless of the order in which the measured data are used:

KAS04: $P_{P1}(RQD > 75\%) = 0.688 * 0.100 + 0.650 * (1-0.100) = 0.654$

KBH02: $P_{P2}(RQD > 75\%) = 0.775 * 0.104 + 0.654 * (1-0.104) = 0.666$

KAS03: $P_{P3}(RQD > 75\%) = 0.732 * 0.104 + 0.666 * (1-0.104) = 0.672$

The entire set of distributions for each updating of the test block is shown in table 5.3 and is graphically displayed in figure 5.2.

Table 5.3. *Prior and posterior distributions for access tunnel block.*

	%RQD=1	%RQD=2	%RQD=3	%RQD=4
Prior	5	10	20	65
after KAS02	5.1	9.0	19.6	66.3
after KAS02 and KAS03	4.7	9.2	19.1	67.0
after KAS02, KAS03, and KAS04	5.1	8.7	19.0	67.2

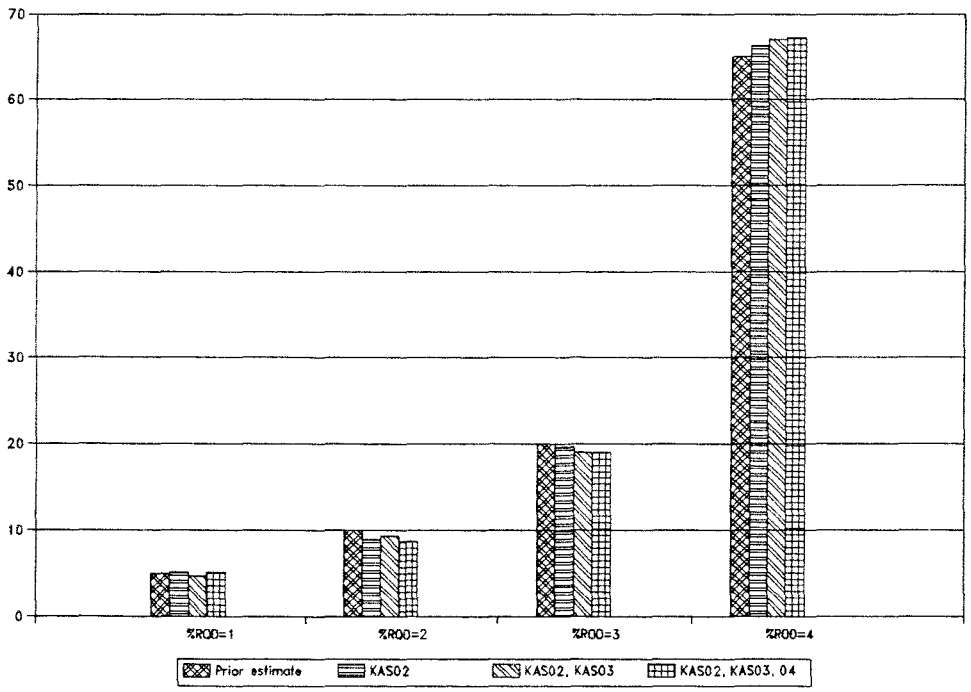

Figure 5.2. *Prior and posterior distributions for the test block. The second column from the left is related to the first used drill core, the third is related to both the first and the second drill core, and so on.*

5.6.2 Access tunnel block

The three drillings KBH02, KAS09, and KAS11 were used for updating in the access tunnel block. The results from the updating procedure in the test block were used as prior estimates. The results are displayed in table 5.4 and figure 5.3.

Table 5.4. Prior and posterior distributions for access tunnel block.

	%RQD=1	%RQD=2	%RQD=3	%RQD=4
Prior	5.1	8.7	19	67.2
after KBH02	8.0	5.8	14.9	71.3
after KBH02 and KAS09	8.6	5.4	14.1	71.8
after KBH02, KAS09, and KAS11	9.2	5.1	13.4	72.3

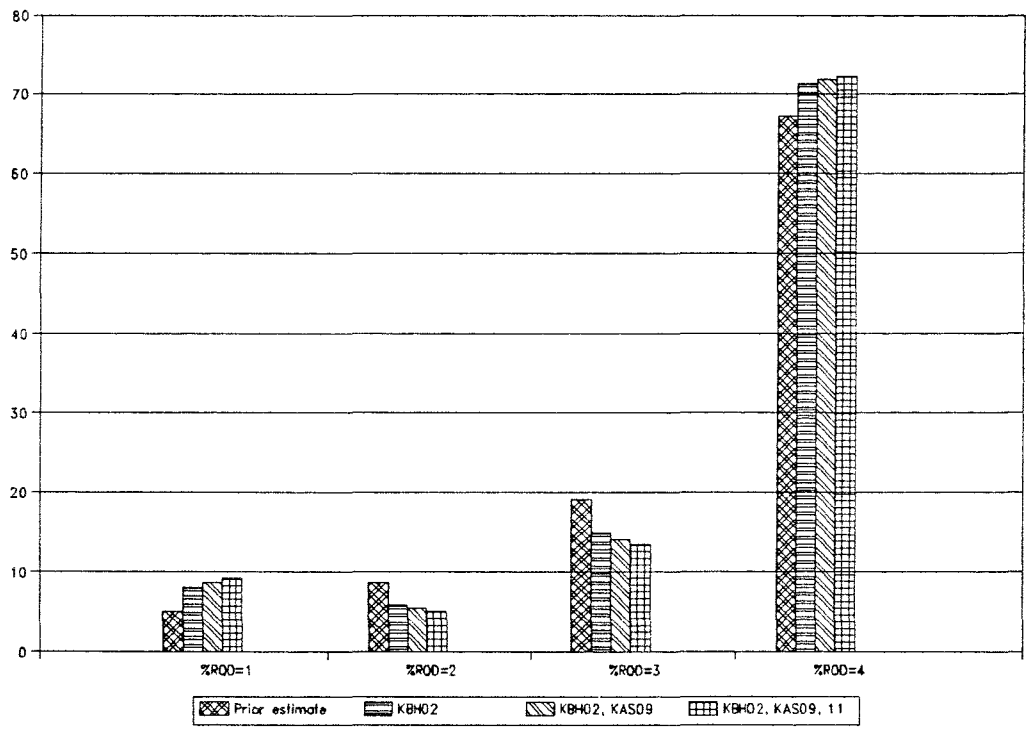

Figure 5.3. Prior and posterior distributions for the access tunnel block. The second column from the left is related to the first used drill core, the third is related to both the first and the second drill core, and so on.

5.6.3 Target block

For the target block the updatings were performed using measurements of drillings KAS02, KAS05, KAS06, KAS07, KAS08, and KAS13. The results from the updating are shown in table 5.5 and graphically displayed in figure 5.4.

Table 5.5. Posterior distributions for target block.

	%RQD=1	%RQD=2	%RQD=3	%RQD=4
Prior	5.1	8.7	19	67.2
after KAS05	4.8	8.4	18.2	68.6
after KAS05, and KAS06	4.6	8.3	17.6	69.5
after KAS05, KAS06, and KAS07	4.6	8.5	16.7	70.2
after KAS05, KAS06, KAS07, and KAS08	4.3	8	16	71.7
after KAS05, KAS06, KAS07, KAS08, and KAS13	4.6	7.7	15.7	72

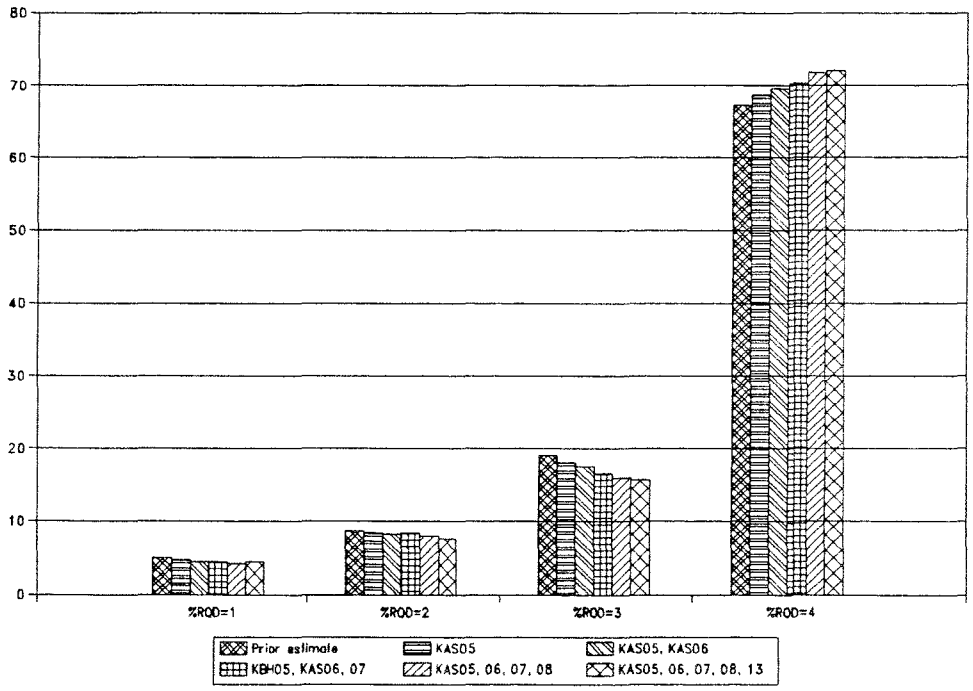

Figure 5.4. Prior and posterior distribitions for the target block. The second column from the left is related to the first used drill core, the third is related to both the first and the second drill core, and so on.

5.7 DISCUSSION

This example was performed in order to display statistical handling and updating of parameters in the suggested classification process using a Bayesian approach. A simple form of Bayesian statistics could be applied since entire volumes of the bedrock were of interest, rather than specific values at certain locations. The latter requires a somewhat more complicated updating approach, since it has to be conditioned with respect to the locations of interest.

The performed example indicated that:

* The prior estimate is of great importance to the result when a small part of the volume of interest is influenced. As more of the volume is influenced, the importance of the prior estimates decreases.

* The order in which the measured data are used has no impact on the final result.

* The influences of the measurements has significant impact on the posterior results, since the influence radius affects the influence volume by the square. Urgently needed is therefore research on autocorrelation in fractured rock, which is a measure of the influence from a drilling. This holds for several of the parameters suggested in chapter 4.

* The Bayesian updating process works well and it is believed that this approach is essential in performing the geoscientific classifications, since it is a relevant approach to integrate and make optimum use of existing data and knowledge. It is suggested that the Bayesian approach is the most relevant way to make optimum use of existing data and knowledge in the classification process.

6 CONCLUSIONS

The purpose of this work was to discuss possible strategies for a geoscientific classification procedure in the siting process of a high-level waste repository in Sweden. It was assumed that the primary interest for geoscientific classifications will be with respect to the safety of the repository. It was also assumed that a in feasible methodology for geoscientific classifications, existing data and professional knowledge should be integrated, which in this report is referred to as a Bayesian approach.

The results of this work can be divided into four major parts:

1. A suggested strategy for identification of areas suitable for geoscientific classifications.

2. A suggested strategy for a classification methodology that is based on a Bayesian approach.

3. A suggested set of critical parameters to be included in the classification methodology.

4. An example of handling of professional judgment and existing data, using a Bayesian approach.

The suggested strategy for identifying areas for geoscientific classifications is based on simple set theory. Areas unsuitable for geoscientific classifications are discriminated with respect to the costs for decisions associated with all factors of interest, geoscientifc as well as other factors, e.g political and demographic issues. It is assumed that the discrimination of unsuitable areas can be performed cost-effectively by making the decisions in sequence with respect to increasing costs, starting with the least expensive decisions. This approach is believed to form a basis for a straightforward identification process that is credible and possible to defend properly.

The classification methodology is based on a classification approach that has been used for different engineering geological purposes, e.g. groundwater vulnerability mapping (the DRASTIC System) and rock mechanical classifications (the RMR System). The suggested methodology has a so called Bayesian approach to allow for optimal integration and use of professional judgments and existing geoscientific data.

A set of critical parameters to be included in the classification system was suggested, based on a literature review of issues important for repository safety. It was the intention to choose parameters that are of importance from an engineering geological point of view, and not for fully describing hydrogeological or geoscientific settings. With respect to the classification validity, resolution, and geoscientific issues of importance to the repository safety the suggested critical parameters are schematically shown in figure 6.1.

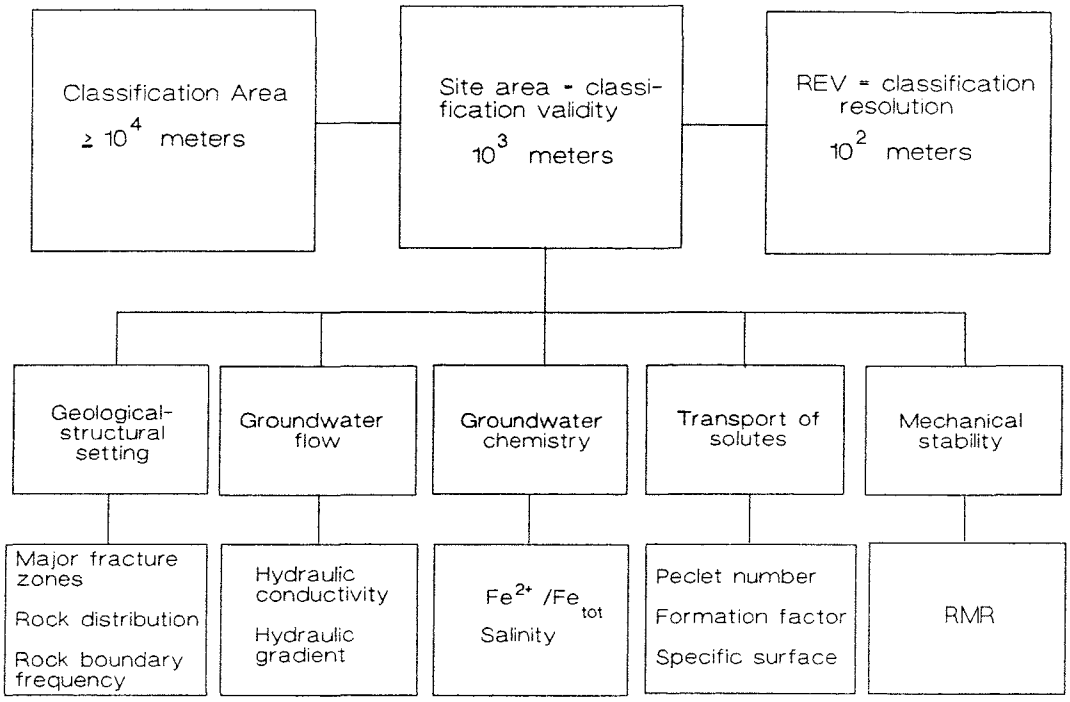

Figure 6.1. Outline of the classification scales, issues and critical parameters.

Several of the suggested parameters need to be further studied to investigate their applicability for the classifications. Research is primarily needed to investigate in more detail how to optimally perform estimations prior to detailed investigations. The set of critical parameters should be regarded as a first-round suggestion that should be further discussed and studied. The final set of parameters should be established through consensus within the geoscientific society. The set of parameters that has been suggested here should thus be revised and updated, if and when that is appropriate.

An establishment of the parameters through consensus would make it possible to credibly defend the classification and siting processes. When the set of parameters have been agreed upon, the discussion regarding the classification results will be directed to the values of the critical parameters. This is fundamental to the siting strategy, since people questioning the classification results will then be questioning the parameter values, and not the methodology. Estimations by different people can be put into the system and it can be studied what these differences mean to the final result. This will tend to bring discussions regarding the importance of different estimations and interpretations of results to a relevant level.

When attention is drawn to the critical parameters, i.e. the criteria that should be fulfilled, the siting process will not focus on comparison of different sites in order to find the best possible site. The objective will instead be a more appropriate one, i.e. to find a good enough site, rather than the best site.

The Bayesian handling and updating of a parameter (RQD) indicated how this approach can give the best estimate possible from existing data and professional knowledge. Poorly understood is, however, what influence different parameters have away from the point of measurement or estimation, i.e. how far parameters can be autocorrelated. Urgently needed is therefore research aiming at analyzing the autocorrelations of the critical parameters, since the results of the Bayesian handling, and ultimately the worth of collecting new data, depend on this. Thus, if a parameter has a very low autocorrelation, it will require a large amount of new measurements to affect the prior estimates and to increase the certainty of the results.

In summary, three main fields of further studies can be identified from this work:

1. To investigate the relevance of the suggested critical parameters in more detail. This means that relevant conceptual models have to be accepted, which should involve further research as well as a consensus procedure.

2. To further study how to estimate several of the suggested critical parameters at repository depths from existing information and knowledge. This is considered to be of primary importance for the following parameters:

    a. rock type distribution
    b. rock boundary frequency
    c. hydraulic gradient
    d. Peclet number
    e. effective specific surface
    f. salinity

3. To study the influence of predictions and measurements on the rock volume of interest, i.e. to analyze the autocorrelations for the critical parameters.

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SKI = Swedish Nuclear Power Inspectorate (Statens kärnkraftsinspektion)
USDOE = United States Department of Energy
USEPA = United States Environmental Protection Agency

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