R-05-33

Äspö Task Force on modelling of groundwater flow and transport of solutes

Review of Task 6C

John Black, In Situ Solutions

David Hodgkinson, Quintessa

March 2005

Svensk Kärnbränslehantering AB
Swedish Nuclear Fuel
and Waste Management Co
Box 5864
SE-102 40 Stockholm Sweden
Tel 08-459 84 00
+46 8 459 84 00
Fax 08-661 57 19
+46 8 661 57 19

ISSN 1402-3091
SKB Rapport R-05-33

Äspö Task Force on modelling of groundwater flow and transport of solutes

Review of Task 6C

John Black, In Situ Solutions

David Hodgkinson, Quintessa

March 2005

Keywords: Keywords: Review of Task 6C, Construction of semi-synthetic hydrostructural model, Äspö Task Force, Modelling, Groundwater flow, Transport of solutes, Site characterisation, Performance assessment.

Abstract

This report forms part of an independent review of the specifications, execution and results of Task 6 of the Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes, which is seeking to provide a bridge between site characterization and performance assessment approaches to solute transport in fractured rock.

The present report is concerned solely with Task 6C, which relates to the construction and parameterisation of a semi-synthetic, block-scale, hydrostructural model of the TRUE Block Scale region of the Äspö Hard Rock laboratory. The task objectives, specifications and outcome are summarised and reviewed. Also, consideration is given to how the hydrostructural model might affect the outcomes of Task 6D and 6E.

Sammanfattning

Denna rapport utgör en del av en oberoende granskning av specifikationerna, utförandet och resultaten från Task 6 av ”Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes”. Task 6 syftar till att bygga en bro mellan ansatser rörande platsundersökningar och säkerhets- och funktionsanalys för transport av lösta ämnen i sprickigt berg.

Den aktuella rapporten behandlar endast Task 6C, vilken i sin tur beskriver konstruktion och parametrisering av en semi-syntetisk, hydrostrukturell blockskalemodell av TRUE Block Scale regionen av Äspölaboratoriet. Syften, specifikationer och resultat har sammanfattats och granskats. Det har även beaktats hur den hydrostrukturella modellen kan komma att påverka resultaten från Task 6D och 6E.

Executive Summary

This report forms part of an independent review of the specifications, execution and results of Task 6 of the Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes, which is seeking to provide a bridge between site characterization (SC) and performance assessment (PA) approaches to solute transport in fractured rock.

The present report is concerned solely with Task 6C, which relates to the construction and parameterisation of a block-scale hydrostructural model of the TRUE Block Scale region of the Äspö Hard Rock laboratory. The task objectives, specifications and outcome are summarised and reviewed. Also, consideration is given to how the hydrostructural model might affect the outcomes of Task 6D and 6E.

The main conclusions of this review are summarised below:

The Task 6C hydrostructural model is a more comprehensive approach to quantitatively describing a volume of fractured rock than has been achieved hitherto. The idea of including solute retention characteristics as indices attached to individual fractures is an efficient device resulting in a whole volume of fractured rock described by a few spreadsheets. The hydrostructural model is clearly defined and provides a useful test bed for Tasks 6D and 6E.

It would have been beneficial if the specifications for Task 6C had been more clearly defined as a hierarchy of requirements, and performance measures had been defined and evaluated to allow comparison of alternative approaches.

The device used to reduce connectivity, namely reducing the average size of background fractures, has the effect of producing a final model with an ‘unnatural’ gap in the overall distribution of fracture sizes.

It appears that the exploratory boreholes could be important conductive structures within the region of the 200 m block even though they are segmented into shorter sections by packers. If correct, this implies that the boreholes should be included explicitly in the model if close replication of TRUE Block Scale test behaviour is desired.

Overall, when compared to the results from the TRUE Block Scale test, the hydrostructural model seems to be too well connected. In this context, it is not clear whether the Task 6C model has been checked for consistency with the hydraulic testing results from the TRUE Block. Scale test area. Whilst it is not the purpose of the Task 6C model to represent the TRUE Block Scale area as accurately as possible, the construction of a model, broadly based on the TRUE Block Scale area, but with too much connectivity, could have the unfortunate result that in Tasks 6D and 6E solutes do not have sufficient time to interact with the rock pore spaces.

Contents

1 Introduction and Objectives

1.1 Context

This report is the second of a number of reports constituting a review of Task 6 of the Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes. The first review report /Hodgkinson and Black, 2005/ is concerned with Tasks 6A, 6B and 6B2, while this report reviews Task 6C.

1.2 Scope and objectives of Task 6

Task 6 seeks to provide a bridge between site characterization (SC) and performance assessment (PA) approaches to solute transport in fractured rock. This is addressed by considering two spatial scales (a single feature and a network scale) and two temporal scales (SC and PA time scales). The two spatial scales are exemplified by the 2.5–10 m pathway lengths of the TRUE-1 tracer tests and the 11–29 m pathway lengths of the TRUE Block Scale tracer tests. The timescales of the tracer tests (i.e. SC timescales) range from a few hours to peak value breakthroughs of up to 40 days. PA timescales are typically in excess of 1,000 years

In Task 6 both PA and SC models are applied to tracer experiments considering both the experimental boundary conditions and boundary conditions of relevance to PA. The approach is firstly to implement models such that they can reproduce the results from relevant Äspö in situ tracer experiments. Appropriate assumptions for PA modelling are then made, while continuing to honour the in situ tracer experimental results.

There is no strict distinction between SC and PA models. However, in general SC models aim to reflect realistic geological complexity and are focussed on phenomena that vary over time scales of less than a year. In contrast, PA models generally adopt simplified geometric assumptions and include slower processes in order to demonstrate with reasonable confidence that repository safety targets are not exceeded over periods in excess of thousands of years.

The objectives of Task 6 have been set out by /Benabderrahmane et al. 2000/ as follows:

1. To assess simplifications used in PA models including:
    a. identifying the key assumptions and the less important assumptions for long-term PA predictions;
    b. identifying the most significant PA model components of a site;
    c. prioritisation of PA modelling assumptions and demonstration of a rationale for simplification of PA models by parallel application of several PA models of varying degrees of simplification;
    d. provision of a benchmark for comparison of PA and SC models in terms of PA measures for radionuclide transport at PA temporal and spatial scales; and
    e. establishment of a methodology for transforming SC models using site characterisation data into PA models in a consistent manner.
2. To determine how, and to what extent, experimental tracer and flow experiments can constrain the range of parameters used in PA models.

3. To support the design of site characterisation programmes to assure that the results have optimal value for performance assessment calculations.
4. To improve the understanding of site-specific flow and transport behaviour at different scales using site characterisation models.

The scope of Task 6 covers seven sub-tasks as follows.

Task 6A models selected TRUE-1 tests in order to provide a common reference platform for all SC and PA modelling to be carried out in subsequent tasks, thereby ensuring a common basis for future comparison.

Task 6B models selected PA cases at the TRUE-1 site with PA relevant (long term/base case) boundary conditions and temporal scales. This task serves as a means to understand the differences between the use of SC and PA models, and the influence of various assumptions made for PA calculations for extrapolation in time.

Task 6B2 is similar to Task 6B except that the boundary conditions are modified to produce flow and transport over a larger area of Feature A. The input boundary is no longer a point source and the tracers are assumed to be collected in a fracture intersecting Feature A.

Task 6C is concerned with the development by a single group of a 50–100 m block-scale semi-synthetic structural model with a hydraulic parameterisation. A deterministic rather than a stochastic model is used so that the differences between models used in later tasks by other groups result from variations in assumptions, simplifications and implementation rather than from the structural framework.

Task 6D is similar in purpose to Task 6A, but is based on the semi-synthetic structural model developed in Task 6C and a 50 to 100 m scale TRUE-Block Scale tracer experiment. This task provides a common reference platform for all SC and PA modelling at the network scale and ensures a common basis for Task 6E.

Task 6E extends the Task 6D transport calculations to a reference set of PA time scales and boundary conditions. The first part of Task 6E uses a basic set of PA and SC assumptions and simplifications while in the second part a sensitivity analysis is carried out by investigating the effects of alternative assumptions.

Task 6F consists of a series of “benchmark” studies on single features from the Task 6C hydro-structural model in order to improve the understanding of differences between the participating models.

The present review is concerned solely with Task 6C /Dershowitz et al. 2003/ which is itself concerned almost solely with Objective 1e.

1.3 Scope and objectives of review

This report forms part of an independent review of the specifications, execution and results of Task 6. The review has been carried out by:

- reviewing background reports on the TRUE programme;
- reviewing the Task 6 specifications, modelling team reports and questionnaire responses;
- participating in Äspö Task Force workshops and meetings; and
- discussions with individual modelling teams.

Task 6C is considerably different to all other sub-tasks in Task 6 in that it has been carried out by one group on behalf of all the other individual modelling teams as a pre-cursor to their efforts in Tasks 6D and 6E. Essentially, a single interpretation of the region of the TRUE-Block scale experiment has been developed. It is expressed in terms of planar features with associated hydraulic and transport properties and is termed a 'hydrostructural' model. It differs from previous 'hydrostructural' models in having transport properties, in addition to hydraulic properties, assigned to individual planar features. There are no 'parallel' or 'alternative' models to compare, so the review procedure is consequently different to that adopted for all the other sub-tasks.

The approach taken in this review therefore is:

1. Review of the Task 6C specification:
   a. does it make sense?
   b. are the objectives clear?
   c. is it well formulated?
2. Does the structural interpretation on which the hydrostructural model is based, seem sensible and is it applied self consistently?
3. Does the representation of the matrix material adjacent to the fracture system seem sensible and is it applied self consistently?
4. Is the outcome of Task 6C, the deterministic hydrostructural model, likely to provide a successful basis for the other groups (with different modelling approaches) to achieve useful outcomes from sub-tasks 6D and 6E?

Obviously, the final element of the review is the most difficult since it concerns a good deal of judgement, particularly about what might be considered a 'useful outcome' from sub-tasks 6D and 6E.

This review takes the view that the hydrostructural model is basically a network of fractures with some system of adjacent matrix material with which solutes flowing through the fractures interact. The review therefore considers first the construction of the fracture system followed by the addition of the various fracture infills and the classification of fracture types.

The 6C report is organised somewhat differently describing first the 'micro-structural elements' (e.g. the matrix materials such as mylonite, cataclasite, fault-gouge etc) (6C Chapter 2), then the construction of the structural model (6C Chapter 3), followed finally by the method used to represent the micro-structural elements as fracture 'complexity' and assign it to the structural elements (6C Chapter 4). It should therefore be borne in mind that this review considers Chapter 2 'out-of order' along with the later parts of Chapter 4, the rest remaining in the order presented in the 6C report.

2 Task 6C specifications

2.1 Objectives and scope

The objectives and scope of Task 6C are provided by /Benabderrahmane et al. 2000/. They are broken down into a set of separate points below and arranged in a slightly different order. The intention is to improve the clarity and separate objective from method. The objectives are essentially:

1. "To develop a 50–100 m block scale synthesised structural model...with a hydraulic parameterisation".
2. This synthesised structural model should use "data from (other Äspö projects) the Prototype Repository, TRUE Block Scale, TRUE-1 and Fracture Characterisation and Classification" projects.
3. The structural model should be "deterministic".
4. "The structural model will include sufficient elements of the TRUE Block Scale experiment to make it possible to reproduce a TRUE Block Scale tracer experiment as part of Task 6D."

These objectives are discussed in Sections 2.2 to 2.5 below.

2.2 Block scale structural model with hydraulic parameterisation

This section considers the objective "to develop a 50–100 m block scale synthesised structural model…with a hydraulic parameterisation".

The first element of the specification, "a 50–100 m block scale model" seems straightforward at first glance. However, most hydrostructural models use natural features, such as the ground surface or large-scale faults, as their boundaries. This is done for obvious reasons, since natural features tend to define both hydraulic boundaries and domains of similar hydrogeological properties. In this case, the region to be modelled is defined only in terms of size. The specification is unclear as to whether the region is a cuboid of 50–100 m edge or a block containing features of 50–100 m extent. Without any pre-defined natural boundaries, it is inevitable that the 50–100 m block will need to be fitted within a larger region in order to identify boundary conditions and limits for the 50–100 m block.

The hydraulic parameterisation of the block scale model that is required by the specification is undefined in terms of what rules should be applied. These are obviously left to the discretion of the team performing Task 6C. It should be borne in mind that the hydraulic parameterisation is extremely important for all subsequent tasks since it fixes all relative water velocities and, together with the boundary heads, also sets absolute velocities.

2.3 Data from other Äspö projects

This section considers the objective that the synthesised structural model should use "data from the Prototype Repository, TRUE Block Scale, TRUE-1 and Fracture Characterisation and Classification" projects.

The specification identifies four previous Äspö projects that the Task 6C hydrostructural model should use for 'data'. It is assumed that the data referred to are characteristics of fractures and their hydraulic performance. The four other Äspö projects are the TRUE-1, Prototype Repository, TRUE Block Scale and Fracture Classification and Characterisation projects. It should be noted that these 4 projects concern very different scales and one is without a significant hydraulic measurement element. The specification does not make clear how these other projects should be used or which forms of data are required.

2.4 Deterministic model

This section considers the objective that the structural model should be "deterministic".

This is understood to mean that all fractures within the modelled block will be defined by Task 6C and that other modelling groups should, at least to start with, use only the 6C defined model as a 'reference case'.

It is apparent from later in the report however that the Task 6C team assume that other groups will be able to adjust the distribution of determined hydraulic parameters in some limited ways, such as organising channels within fracture planes. One assumes that this is inevitably necessary where other groups are not using models based on planar features.

2.5 Possibility of reproducing TRUE Block Scale tracer experiment

This section considers the objective that "the structural model will include sufficient elements of the TRUE Block Scale experiment to make it possible to reproduce a TRUE Block Scale tracer experiment as part of Task 6D."

In reality this is probably the most definitive element of the specification because it gives an indication of how the hydrostructural model might be assessed. It seems unfortunate that some 'reference' outcomes are not included within the deliverables of Task 6C, but rather is left to the other groups performing Task 6D using their own models.

It is suggested that if this is truly regarded as a measure of the success of Task 6C that some initial simulations of the TRUE Block Scale tracer experiments should have been included within Task 6C. As it is, the reader is left having to make some assessment of whether the hydrostructural model produced by Task 6C will be suitable for Tasks 6D and 6E when used for a wide range of modelling approaches.

2.6 Additional specifications

Up to this point the specifications for Task 6C lack detail. They appear to be a summary of some quite detailed discussions that occurred at Goslar in September 2001 and at Thoresta Herrgård 6 months later. These discussions are more completely described in Section 1.5 of the Task 6C report under the heading, "Selection of a prototype for the Task 6C semi-synthetic hydrostructural model" and are referred to as "decisions and guidelines". They are:

- Focus on a rock volume 200×200×200 – m in size centred on TRUE Block Scale (larger volume included for completeness).
- Account for observed compartmentalisation /length scale of connectivity for the included deterministic structures.
- Generate structures based on available statistics.
- Retain elements of site scale model (i.e. very large scale) of Äspö HRL.
- Update report disposition, i.e. emphasise integration of information …in various reports, unification of terminology, produce clarifying figures.

A further specification occurs within a discussion of possible candidates for a starting point for the hydrostructural model mentioned earlier in Section 1.5 of the Task 6C report, namely:

- "...the deterministic hydrostructural model (of the prototype repository) consists of only 2–3 sub-parallel, vertical structures…….insufficient to form a conducting network of deterministic features; hence block-scale connectivity can only be achieved using stochastic background fractures. This condition is inconsistent with the premises for Task 6C, which require a basic network of deterministic features."

Consequently one of the detailed specifications of Task 6C is that the hydrostructural model should include some specified features, more extensive than background fractures that interconnect at the block scale.

This is an important requirement because there is a potential conflict between specifying a connecting network of features/fractures on a scale of at least 50 m, and satisfying the requirement to "account for observed compartmentalisation for the included deterministic structures".

2.7 Summary

At first sight, the specifications for this task lack detail. However, there are a considerable number of detailed requirements that the model should attempt to meet. Some of these don't appear to be easily reconcilable with each other. Thus some form of prioritisation might have been useful. Additionally some of the specifications are either 'shorthand' for a complicated concept (e.g. account for observed compartmentalisation for the included deterministic structures) or are summaries of a detailed discussion (e.g. retain elements of site scale model). It would have been helpful if the more detailed requirements had been described more fully and explicitly, including a discussion of what they were designed to achieve.

The objectives and requirements described in Section 1 of the Task 6C report constitute a complex series of ideas. It would have been useful to have collected all the various objectives and requirements together in a single section of the Task 6C report and to have presented reasoned arguments as to how they should be prioritised. Such a section could also have usefully identified some performance measures, preferably some of which could have been evaluated within Task 6C rather than in Tasks 6D or 6E.

3 Enhanced hydrostructural model

In order to meet objective 4 (Section 2.1), namely to make it possible to reproduce a TRUE Block Scale tracer experiment as part of Task 6D, Task 6C developed a unique ‘enhanced’ hydrostructural model. It is ‘enhanced’ in the sense that, unlike previous hydrostructural models such as that applicable to the TRUE Block Scale project and summarised in /Poteri et al. 2002/, it assigns characteristics pertinent to solute retention to all included structural features.

This is a significant step and involves, in this implementation, the development of a pair of indices, ‘geologic structure type’ and ‘complexity factor’. Because these are thought to be dependent on feature size, there is also the need to develop scaling rules. Consequently this ‘enhanced’ hydrostructural model is a complex intellectual construct.

It would have been valuable to the reader if the report had included a broad description of the overall philosophy used to specify the model and in particular which elements are entirely deterministic and which have a probabilistic component. For instance, the so-called deterministic structures of the TRUE Block Scale (e.g. Structures 5–24) are placed in space on the basis of observed conductive intersections in boreholes, but are extended beyond known intersections on the basis of an overall size distribution.

The eventual model contains the major structures identified in the TRUE Block experimental area plus the large-scale structures of the ‘site-scale’ investigations. These are all structures that have been ‘determined’ as a result of experimental observations. In addition, the hydrostructural model includes a population of small-scale (background) features that are generated by a Discrete Fracture Network (DFN) model of the TRUE Block experimental area. There are also some extra ‘mid-scale’ features (~ 100 m) that belong to a second population and are generated to ‘fill in the uninformed parts of the 200 m scale model’. Hence some elements of the eventual ‘enhanced’ hydrostructural model are a product of the assumptions inherent in DFN modelling.

It should be borne in mind that DFN modelling, as used in this work, entails the important assumption that fractures are roughly equi-dimensional. This has important implications for connectivity.

4 Is the model constructed self-consistently?

4.1 Summary of approach

The detailed approach to Task 6C is outlined in Section 1.6 of the report /Dershowitz et al. 2003/. It is briefly summarised below with some additional description.

The Task 6C semi-synthetic hydrostructural model is based primarily on the March 2000 hydrostructural model of the TRUE Block Scale Experiment put forward by /Hermanson and Doe, 2000/. The modelled region is a cube with a 200 m edge. The original '2000' model contained 24 'structures' whose location and properties were identified through interpretation of a wide range of geoscientific observations, and not just on the results of the tracer tests. Based on an additional analysis of site data within the Task 6C project, 13 of the original 24 'structures' were eliminated. The resultant '11 structure' model is itself located within a much larger region, the 'site-scale model' which is a rectangular region, 2 km × 2 km in plan by 1 km deep (Figure 4-1). The larger region is the so-called Äspö Task 5 hydrostructural model of /Rhén et al. 1997/ and contains 22 large-scale structures.

The smaller 'block-scale' region has been characterised using boreholes and underground excavations that do not sample the region homogeneously. Hence the deterministic structures are not evenly distributed. To solve this problem, a further 25 '100 m scale' structures were introduced within the 200 m block according to a spatial model based on the 11 deterministic structures.

A further level of fracturing was also synthesised: the so-called 'background fracturing'. Background fractures were considered to be less than 50 m scale and were also inserted into the 200 m region according to a set of procedures concerning density, orientation, extent etc 5,660 background fractures were generated to populate the 200 m block.

This process of structure and fracture synthesis was repeated for the whole 2,000 m block using the same approach as had been developed for the 200 m block. A further 46 mid-scale (100 m) structures were included in the site-scale model.

It was considered that the origin of fractures has a major impact on the types of minerals that are found within them and therefore a strong influence on their solute retention characteristics. Two types of conductive feature (fracture) were identified: fault related (Type 1) and non-fault related (Type 2).

The microstructural model of Type 1 features envisages fractures containing various assemblages of mylonite, fault gouge and cataclasite in addition to the Type 2 combination of intact matrix rock, hydrothermally altered matrix rock and mineral coatings. Procedures were constructed to define which features are assigned to be Type 1 or Type 2 but, in general, larger features are considered more likely to be fault related and so were assigned the geometry and mineralogy of Type 1.

The outcome of Task 6C is a set of spreadsheets defining 3 groups of fractures/structures (background, mid-scale (~ 100 m) and 'site-scale' (~ 1,000 m)) in terms of their geometry, transmissivity, complexity and microstructure.

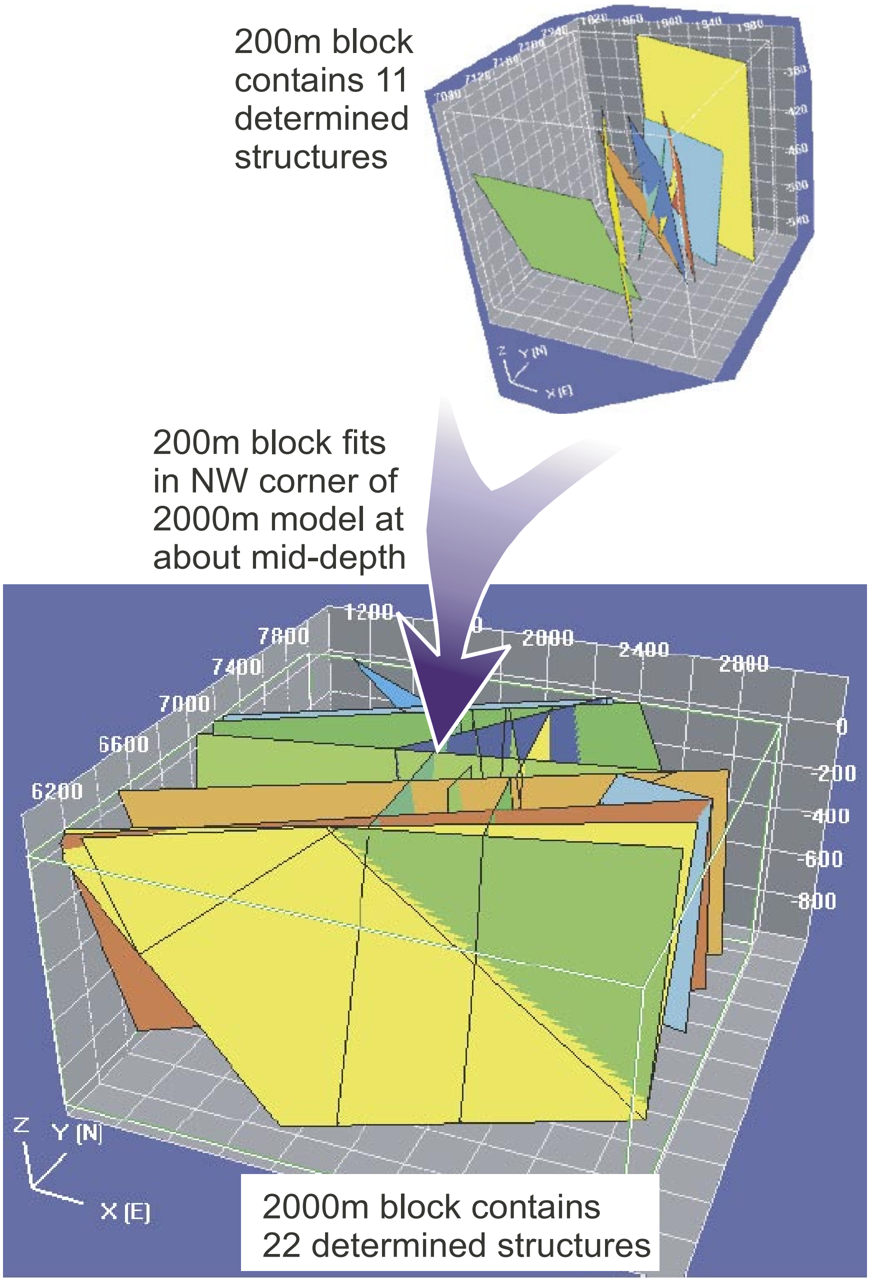

Figure 4-1. *Schematic illustrating how the basic hydrostructural model contains 33 determined structures.*

4.2 Terminology

The DFN approach underpins the structural interpretation of Task 6C. It is used to analyse the existing information, deduce procedures for populating a region with fractures and then to generate fractures stochastically to fill the two chosen regions. The fractures that are generated are defined in terms of the location of their 4 (sometimes 5) corner points and are single planes.

In contrast, much of the report refers to "structures" and "features" as well as "fractures". At times these terms seem to be used interchangeably and the various definitions included in the report add to the confusion rather than resolve it. Thus:

In Section 3.2: Definition: A background fracture is ....defined as a feature of scale less than 50 m......and can be made up of one or more discrete features.

In Section 1.6: An empirical 'complexity factor' is introduced to quantify the variation in... the number of fractures or features which make up a structure at a given scale.

In Section 3.3.1: The primary conductive elements of the 200 m scale...model are the interpreted deterministic...structures.

In Section 4.1: For each synthetic structure, the properties of the structure depend on the size of the structure. .....assign properties using a correlation to fracture size.

In Section 4.2: The intensity P_{32} specified for 100 m scale structures is 0.02 m^2/m^3. The intensity P_{32} specified for background structures is 0.29 m^2/m^3. These structures are generated within the model region until this level of intensity is reached.

For both 100-m scale structures and background fractures......locations are generated as points on the surface of the structure...

The reason why this is important is because one of the basic indices of a fracture network is its fracture intensity (P_{32}) and this needs to be honoured when fractures are generated for the eventual hydrostructural model. From the definition in Section 3.2 (see above), the basic element of the hydrostructural model is a 'feature'. These are combined to form 'structures', that range in size from 'background fractures' to '1,000 m scale structures'.

It is also clear from the text in Section 4.2 (see above) that the FracMan code is used to generate 'structures' and defines them as planar surfaces. If the structures comprise 'multiple discrete features' (see Section 1.6 and above), then what is calculated as a 'fracture intensity P_{32}'? It seems from Section 4.2 that the P_{32} relates to entire structures.

The question recurs through the introduction of the concept of 'structure complexity' (6C Section 4.4.2). It would appear that individual 'structures' defined in the Task 6C report have been allocated a complexity factor that itself defines how many features/fractures (using the nomenclature of the report) make up a 'structure'. The use of the complexity factor is explained in Section 4.4.2, thus:

Ideally, each of the conductive features/fractures that make up the structure should be specified explicitly, complete with its geometric, hydraulic, transport and geologic properties. This level of detail, however, is well beyond the scope of Task 6C, even for the interpreted deterministic structures. Instead, a simplified system has been adopted in which the number of conductive features/fractures.........is specified by a "Complexity Factor".........A complexity factor of 3 implies 1–3 parallel fractures along the extent over which 50-90% of the outline (and associated fracture area) are associated with the primary structure type given in Table 4-5........ In this simplified model, the distance between near parallel features/fractures within a single structure is assumed to be 0.2 m based on available data and observations.

Within this explanation there are some points of concern. First ‘features’ and ‘fractures’ appear to be interchangeable, effectively contradicting the definition in Section 3.2. Possibly of more concern is; if conductive features are generated according to a procedure regarding fracture intensity, how is this rule honoured when the assignment of a complexity factor to a particular structure, post-generation, can generate a further group of sub-parallel fractures (up to 10+ for Complexity Factor 5) each one 0.2 m from the next? One assumes that this problem is minimised by the assignment of extra fractures according to structure extensiveness (6C Table 4-9) so that only structures in excess of 100 m have complexity factors in excess of 3 (i.e. > 3 (sub-parallel) conductive features/fractures per structure). Since the more common structure sizes have less than 3 extra sub-parallel fractures the deviation from the stated intensity is probably minimal.

For the future it is recommended that the members of the Äspö Task Force develop and use agreed definitions for ‘fractures’, ‘features’, ‘structures’ and possibly other terms that are commonly used in fracture flow and transport modelling.

4.3 The basic fracture network descriptors

Five basic parameters are used to define a water-conducting discrete feature in the hydrostructural model. They are ‘orientation distribution’, ‘intensity’ (P_{32}), size equivalent radius, fracture transmissivity and spatial pattern. The orientation data are unambiguous and are straightforwardly implemented within the hydrostructural model. The other four parameters are considered below, firstly for ‘background fractures’ and then for ‘100-m scale structures’ as per the order in the report. In this part of the review, we use the term fractures to denote the basic planar elements that are used in the ultimate model.

4.3.1 Background fractures

The basic difficulty with any analysis of fractured rock and its representation as a discrete fracture network (of only the conductive fractures) is that not all of the fractures that can be observed as a trace map can possibly conduct water. The identification of conductive fractures is usually based on the results of single borehole hydraulic tests. In the case of the TRUE Block Scale region the hydraulic tests include selective packer tests and comprehensive flow logs, including ‘Posiva flow logs’. These tests do not assess hole-to-hole connection so each flow ‘anomaly’ is treated as an individual fracture. It should also be borne in mind that since it depends on borehole intersections the orientations of the boreholes have a major effect on the sampling.

Four boreholes were used to derive the statistics on background fractures reported in /Andersson et al. 2002/. They cover a slightly limited array of orientations (see Figure 4-2) and are poor samplers of any fracture or feature with a SW to NE strike.

A statistical analysis was performed on the flow anomalies remaining after removing those associated with the determined (100-m scale) structures. This yielded 2 conductive sets of fractures both with log normal distributions of size with mean equivalent radii of 6 m (and a standard deviation of 3 m) but slightly different intensities, 0.16 m^2/m^3 and 0.13 m^2/m^3. Both sets were also interpreted to have the same transmissivity distribution with a mean value of 1.1×10^{-9} m^2/sec.

The interpretation of spatial pattern was based on the intersection frequency of the flowing features with the same 4 boreholes and evaluated against 21 different possible distributional forms. In the end, where information was most dense, in the region of the

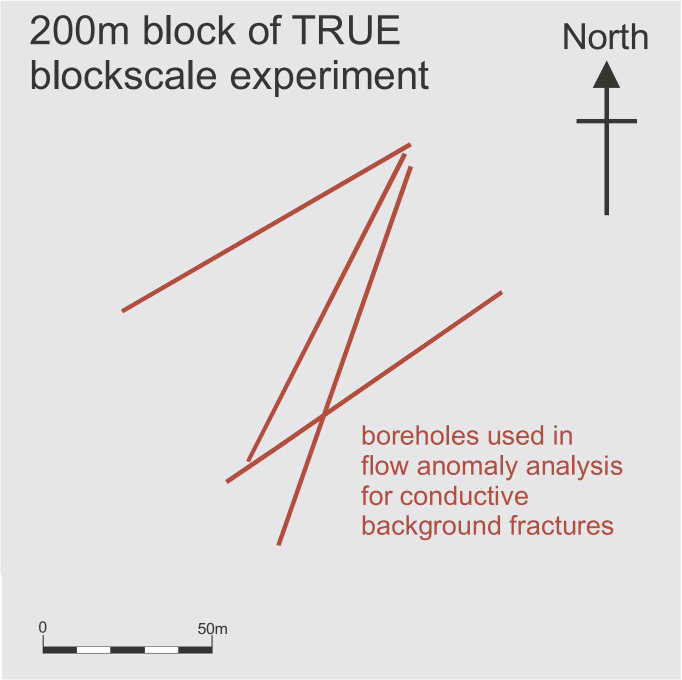

***Figure 4-2.** The orientations of the boreholes used to derive information on the frequency and orientation of conductive fractures in the 200 m TRUE Block Scale region.*

TRUE Block Scale tracer tests, the fractures were interpreted as being Poisson distributed in space (the 'Baecher' model) and fractally organised in the rest of the 200 m block.

These results are all from the report by /Andersson et al. 2002/ but when they were used in /Dershowitz and Klise, 2002/ to simulate crosshole interference tests, it was found that simulated tests had too many responses. In other words the network based on the analysis was too well connected.

The response of the authors of Task 6C was to assume that the interpreted mean conductive fracture size was too large and to reduce it from the 6 m mean value taken from /Andersson et al. 2002/ to a value of 2 m (and a standard deviation of 1 m). The justification for this reduction is, according to the text, that the original 6 m value is based on a study by /Follin and Hermanson, 1997/ in the TBM tunnel and that: "Considerable data from other areas in the Äspö tunnels supports size distributions for background fractures with average sizes more on the order of 1 to 2 m……". It goes on to say that the recommendation of 2 m is based on "data from the adjacent Prototype Repository rock block /Hermanson and Follin, 2000/ and the FCC project analyses /Mazurek et al. 1997/".

This is confusing because /Anderson et al. 2002/ attribute the characteristics of their hydrostructural model to /Hermanson and Doe, 2000/, which is based on borehole KI0025F03 within the TRUE network block and, by inference, their statistics on background fractures. The rest of Section 3.2 contains some confusing references and it is not entirely clear which projects influenced the choice of size of the background fractures.

The work by /Bossart et al. 2001/ concentrated on an examination of small-scale structures and an evaluation of how the observation of fracture traces influenced the ultimate DFN model parameters. Mean sizes of three different possible networks ranged from 0.15 to 0.5 m so 2 m might be an overly high estimate for the mean fracture size. To some extent, the work by /Bossart et al. 2001/ is a reminder of how much variability is possible when the same data set is interpreted using different concepts.

The authors of Task 6C, having reduced the mean size of background fractures from 6 m to 2 m, retain the original values of fracture intensity of 0.29 m^2/m^3 and mean transmissivity meaning that the number of fractures generated increases. It is noteworthy that the mean value of fracture transmissivity at 1.1×10^{-9} m^2/sec is only just above the stated threshold of 1.0×10^{-9} m^2/sec with a standard deviation of 0.93 log cycles.

After changing the mean size of the background fractures to reduce connectivity, it appears from a remark beneath Table 3.2 that the outcome of this change was not checked against the aforementioned crosshole interference tests.

4.3.2 100 m scale structures

The basic idea described in the Task 6C report concerns the identification of some 100 m scale deterministic structures as a group in order to then define their collective geometric and transmissive properties so as to enable a similar group to be introduced to fill the regions where measurements are sparse or non-existent. This yielded a single set with their strikes aligned close to NW-SE and randomly distributed (i.e. Poisson) in space. They had a log-normal distribution of sizes with a mean diameter of 108 m (standard deviation of 55 m) and a fracture intensity (P_{32}) of 0.02 m^2/m^3.

Structures are treated as planar and are each assigned a single value of effective transmissivity that is the geometric mean of all the single borehole measurements where the structure has been intersected. Most of the structures listed in Table 3.5 of the Task 6C report have yielded transmissivity distributions with a standard deviation of about half a decade. The text makes it clear that varying transmissivity in the plane of the structure will be one of the “more realistic variations” performed by the other teams. The use of the geometric mean implies no specific organisation in the structure.

4.3.3 1,000 m scale structures

It is assumed that all 1,000 m scale structures are known and fully characterised (see Figure 4-1) and therefore no synthetic structures need to be introduced at this scale. A certain amount of flexibility is built in by the assignment of large complexity factors to the large-scale structures so that these large structures may include many sub-parallel fractures.

4.3.4 Summary

Although the proposed hydrostructural model is deterministic in the sense that every structure is defined, some of the model’s elements are based directly on field evidence and some indirectly. At the most detailed level, background fractures are described and located everywhere on the basis of a DFN interpretation. At the next scale up, the 100 m scale, some structures in the centre of the TRUE Block Scale experiment are known and are therefore defined directly. Because information is not evenly distributed throughout the region, a group of additional 100 m scale structures are created on the basis of an interpretation of the structural arrangement of the directly determined structures. On the largest scale a few 1,000 m scale structures are defined deterministically. Although all three populations coexist in the same region, from the statistics provided in Tables 3.1 and 3.7 of the Task 6C report, the smaller two are quite different. Background fractures include two predominant orientations whereas 100 m scale structures have only one. The only aspect they have in common is that the distributions of size and transmissivity are both log-normal.

Whilst this may not seem noteworthy at first glance, it implies that the conductive features are a differently orientated subset of all features dependent on scale. It is not clear in the account of Task 6C whether such relationships are present in the data, are the result of sampling bias or whether the rules that apply for the interpretation of background fractures cease to apply at some particular scale when conductive structures are analysed.

Defining these groups on the basis of scale seems like an important step but the choice of scale is not discussed. Further concern is generated by the authors' response to some initial assessments of background fracture connectivity, where their response was to reduce fracture diameter to one third of their original estimate whilst retaining the original intensity. The justifications in the text are not entirely clear.

4.4 Assignment of properties to synthetic structures

There are two main elements to the assignment of properties to the synthetic structures, the choice of transmissivity value for each structure and the choice of a 'microstructural' model.

4.4.1 Assigning transmissivity to structures

This section of the report has the same problem of terminology as the rest of the report in that the words 'fracture', 'feature' and 'structure' are used interchangeably. It is a particular distraction in this section since structures are obviously made up of individual fractures and yet they are analysed as if they have a collective behaviour. This ambiguity is of particular concern in the next section dealing with the use of the 'complexity factor'.

Returning to the assignment of transmissivity, the report discusses very briefly the concept of there being a correlation between fracture size (used here to signify extensiveness not width) and transmissivity. In other words, more extensive fractures are more transmissive. The report provides an Äspö based diagram illustrating the correlation (Figure 4-1 of the report is reproduced as Figure 4-3 below).

As the Task 6C report explains, the figure contains a mixture of deterministic and probabilistic results. The 'TRUE BG' data points are output from the hydrostructural model relating to background fractures in the TRUE- Block Scale region. The text says they are based on Table 3-1 but Table 3-1 has a mean value of 6 m whereas the data points look to have more like a 2 m mean (the mean size was decreased to reduce connectivity). The original value would shift the whole group to the right by half a log cycle. The TRUE BS data points are the deterministic structures of the TRUE Block Scale region, which include an interpretation of the size of each structure and an assignment of transmissivity based on the geometric mean of field measurements. There are however 18 data points in the figure corresponding to the reference, /Andersson et al. 2002/, whereas the Task 6C authors have earlier reduced the number of deterministic structures to 11 (and listed in Table 3-5). The final group is also based on field measurements, apparently cross-hole determined transmissivity values. A minor uncertainty about this diagram is how the choice of the number of background fracture data points to include in the correlation may influence the derived relationship since the other two scales are limited in number.

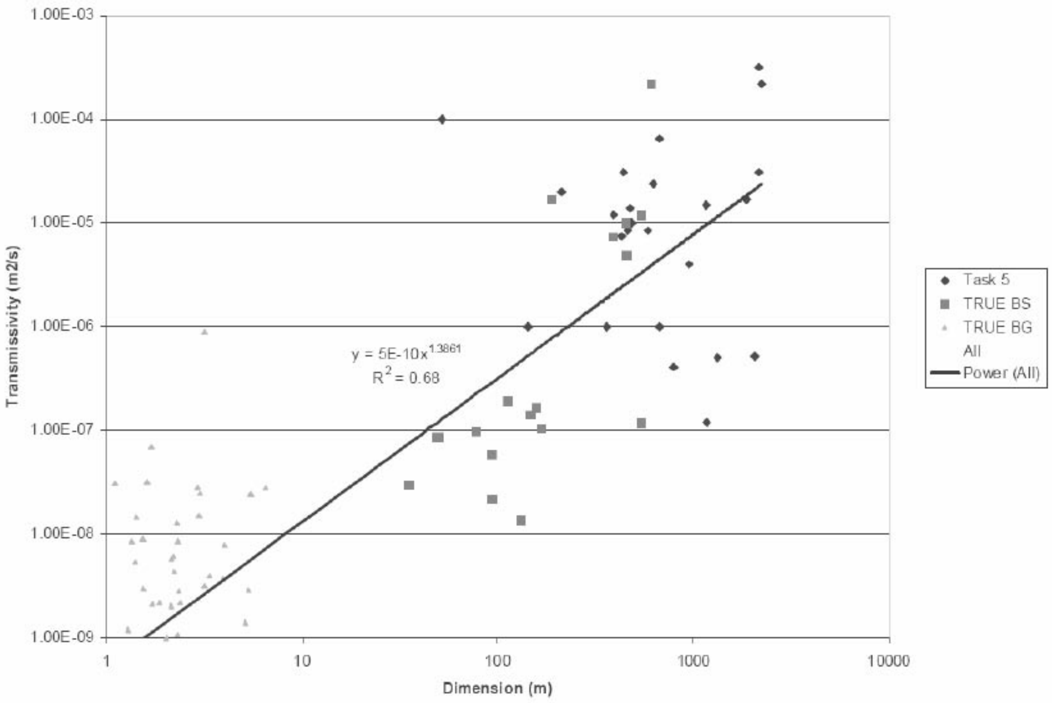

Figure 4-3. Correlation between structure/fracture size and transmissivity (copy of Figure 4-1 of Task 6C report).

The diagram also serves to highlight the question of the choice of three distinct scales in that the two larger scales obviously overlap whereas, according to the diagram, the hydrostructural model of Task 6C contains no fractures/structures/features in the size range between about 7 and 30 m. This 'gap' is probably caused by the previous decision to reduce the mean size of background fractures by a factor of 3. This 'gap' is a consequence of the attempt to increase compartmentalization and seems somewhat 'unnatural'.

Another aspect of these groups of data is the question of connectivity. In common with the background fractures group, the summary of the TRUE Block Scale experiment /Poteri et al. 2002/ states that there were problems of over inter-connection between the determined structures in the Block Scale hydrostructural model. One of the solutions was to stop structures 13 and 21 connecting at their intersection (page 190 top paragraph). There were also over-connection problems for the largest scale structures, and in the report by /Rhén et al. 1997/ the structures are given a skin to stop them allowing too much flow into the underground openings. In other words there is evidence at all scales of the hydrostructural models over connecting. Although, the problem has been approached in the Task 6C project by making the background fractures smaller, this has not been done for the larger scales, and a result is a rather unnatural distribution of fracture sizes.

It should be borne in mind that one of the assumptions of the DFN analysis and subsequent model reconstruction is that fractures are equi-dimensional. Removing this assumption would have a significant impact on connectivity.

In summary, within Task 6C it is assumed that the transmissivity of fractures increases as they increase in size according to the equation:

Transmissivity = $5\times10^{-10}\times L^{1.386}$,

where L is fracture diameter.

Obviously there is a degree of variability and a correlation coefficient of 0.68 was proposed.

4.4.2 Assigning microstructural models to structures

The Äspö approach to microstructural modelling has been developed over a number of years, and identifies characteristics of structures related to their origin either as fractures without evidence of shear (Type 2) or fractures with evidence of shear (Type 1). The steps in assigning the characteristics are:

1. Assign structure type – Type 1 or Type 2;
2. Assign 'complexity factor';
    - the typical number of conductive features that make up a structure;
    - the variation in the number of features comprising the structure at different locations in the structure;
    - the variation in feature 'type' amongst the features.

The Task 6C report begins by establishing a relationship between structure type and structure size. Larger structures were considered more likely to be Type 1 structures (i.e. with associated shear) than smaller ones, which seems reasonable.

The complexity factor clearly has a significant effect on the nature of a feature and on its geochemical behaviour. The Task 6C report describes the derivation of a relationship between complexity factor and structure size illustrated in Figure 4-4.

One of the essential aspects of the complexity factor is that it recognises that large-scale structures comprise many fractures and it does this by including extra fractures into the model. The numbers and their meaning are defined in Table 4-5 of the Task 6C report (reproduced as Table 4-1 below).

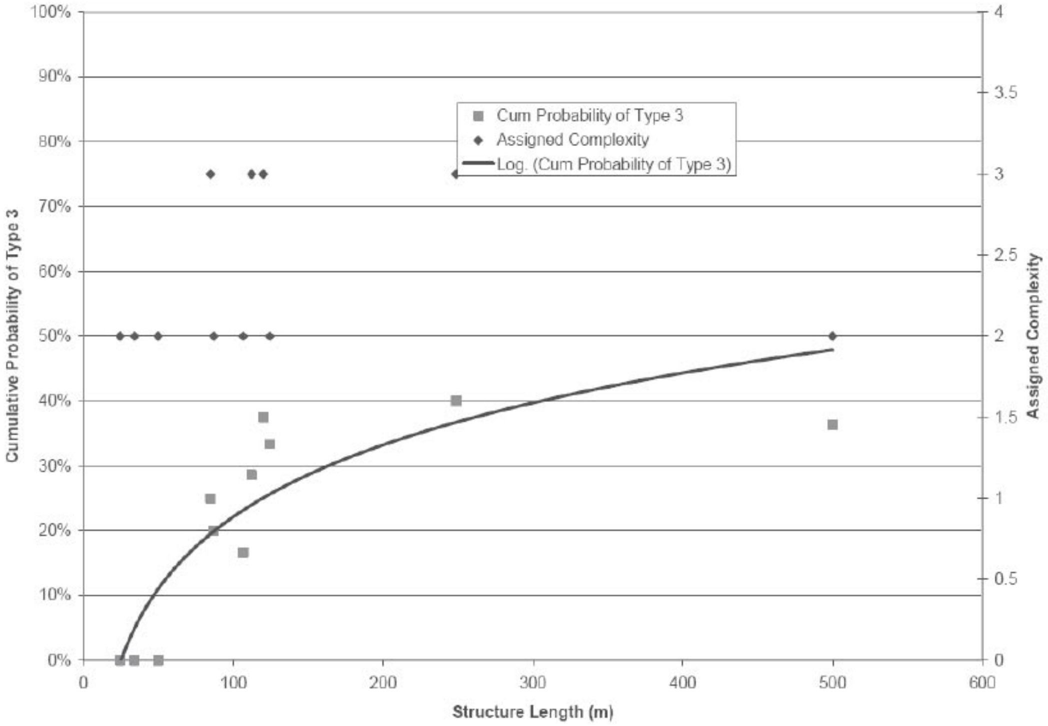

Figure 4-4. Relationship between complexity factor and structure size for TRUE Block Scale deterministic 100 m scale structures (copy of the Task 6C Figure 4-6).

Table 4-1. Definition of complexity factor assigned to modelled synthetic structures (copy of Table 4-5 of Task 6C report).

Complexity Factor	Number of (sub-parallel) conductive features/fractures per structure	Percent of primary geological structure type or combination of geological structure types (by area)
1	1	90–100%
2	1 to 2	70 to 100%
3	1 to 3	50 to 90%
4	3 to 10	50 to 90%
5	10 +	50 to 90%

The assignment of a microstructural model is a useful method of simplifying a complex configuration. In the future development of this concept, the following questions should be addressed.

1. How will we ever know what element of the microstructural model is most important for retardation; mineral composition, internal structure feature frequency, etc? It has to be assumed that these influences will be separated by sensitivity studies.
2. If the 'complexity factor' introduces extra features/fractures into the model, after the fracture intensity has been fixed in the model generation process then how well will the chosen P_{32} be honoured by the ultimate model?
3. If the 'complexity factor' is applied at all scales including background fractures then what is the basic unit of generation, is it features because background fractures are made up of features?
4. The microstructural model includes such elements as the thickness of all mineral zones (i.e. intact wall rock, altered zone, cataclasite, etc) and the distance between adjacent fractures. How is consistency maintained so that some volumes of the modelled region are not assigned more than once?

It can be concluded that the resulting model is difficult to check for consistency.

4.5 Boundary conditions

Boundary heads need to be assigned to the hydrostructural model for use in modelling both the TRUE Block Scale tracer tests as well as long-term nuclide migration. The approach used in the Task 6C (Section 1.6) was to "use hydraulic head boundary conditions such that explicit geometric modelling of tunnels and shafts can be avoided". The boundary conditions for the 200 m scale block are illustrated in Figure 6-1 of the Task 6C report.

For the purposes of this review the two images have been edited and rearranged in Figure 4-5 below together with a 'perspectivised' map of the plan of the boreholes within the block. They are moved outside the block region for the purposes of clarity. The main tunnels of the Äspö HRL lie to the north east of the block and are obviously a low head region. It is clear from Figure 4-5 that the low head of the main Äspö tunnels is propagated across the TRUE Block region by the exploratory boreholes since there are no 100 m scale features aligned in the N-S direction (see Task 6C report Figure 5-4). It would seem therefore that the exploratory boreholes are important conductive structures within the region of the 200 m block even though they are segmented into shorter sections by packers. If correct, this implies that the boreholes should be included explicitly in the model.

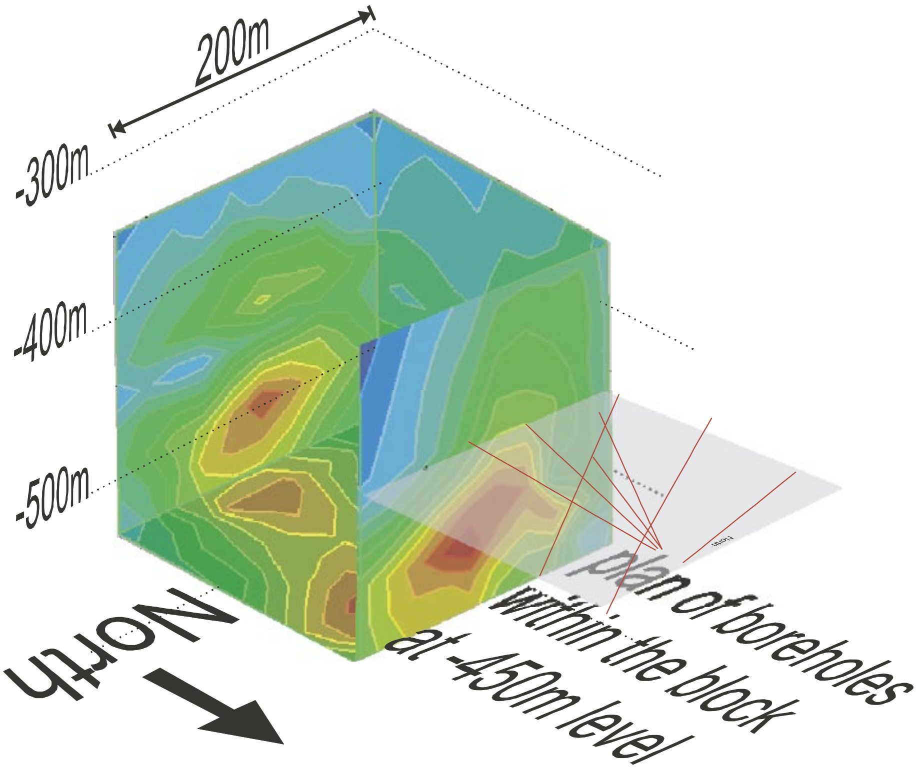

Figure 4-5. *Head conditions to be used on the surfaces of the 200 m block. N.B. red is low head, blue is high.*

5 Conclusions and recommendations

5.1 Overall conclusions

The Task 6C hydrostructural model is a more comprehensive approach to quantitatively describing a volume of fractured rock than has been achieved hitherto. The idea of including solute retention characteristics as indices attached to individual fractures is efficient meaning that a whole volume of fractured rock is described by a few spreadsheets. The approach also includes an explicit size dependence for the retention properties, which is fit for purpose, namely as input to Tasks 6D and 6E, but should continue to be investigated further.

The main shortcomings of the model are its likely over-connection and thereby unrealistic throughflow times. In this context, it is not clear whether the Task 6C model has been checked for consistency with the hydraulic testing results from the TRUE Block.

5.2 Task 6C specification

Task 6C aims to construct a hydrostructural model that would allow other modelling groups to model a ‘standardised’ region. This is actually much more difficult to define than might be thought. It is clear from the text of the Task 6C report that the specifications were formulated gradually at a number of meetings and discussions. The actual specification is minimal. Many of the underlying guidelines and requirements appear gradually as one reads the Task 6C report.

The ideas and general considerations underlying the model are just as important as the hydrostructural model itself. The requirements, particularly what it has to be able to achieve by way of matches to field measurements, should have been made more explicit. Also the aims should have been prioritised so that where they are in conflict, the more important requirements could have been seen to be met at the expense of the less important.

In addition, it would have been useful if some performance measures had been defined to facilitate comparisons among different approaches to meeting the specifications.

5.3 Is the DFN approach applied self consistently?

The DFN approach is used to generate the background fracture system. It has a number of implicit assumptions and it is not clear that they are all adhered to when the background fractures were adjusted. For instance when it was decided that the model was over-connected and the mean diameter of the individual features was reduced from 6 m to 2 m, was it realised that the underlying assumption of the conducting features being a representative sample of all features was being dispensed with? The associated outcome seems to be a system of fractures that contains an unnatural gap between 7 m and 30 m fracture size.

An alternative to reducing the diameter of fractures would be to relax the assumption that fractures are equi-dimensional, which would have a significant impact on connectivity.

The specifications appear to include some potentially conflicting requirements. Is it really possible to produce a hydrostructural model that, on the one hand, contains a system of interconnecting major structures and yet also produces compartmentalisation of heads and nuclide transport?

The model is built with the assumption of scale-related characteristics applying to some major characteristics namely transmissivity and microstructural model. While this is fit for the intended purpose of forming a basis for Tasks 6D and 6E, these relationships are not necessarily correct and should not be used in other contexts without further justification.

The question of the incorporation of the boreholes as one of the major structural elements of the hydrostructural model is intriguing. The head field seems to call into question the very nature of the predominant feature orientation, and possibly points to there being an insufficiently varied set of borehole orientations.

5.4 Is the representation of the microstructural model sensible?

The microstructural model is a useful method of simplifying a complex configuration, and the approach of using a complexity factor is an interesting approach to reproducing realistic variability with the minimum of computational effort. However, in future developments of this concept, the following questions should be addressed.

1. How will we ever know what element of the microstructural model is most important for retardation; mineral composition, internal structure feature frequency, etc? It has to be assumed that these influences will be separated by sensitivity studies.
2. If the ‘complexity factor’ introduces extra features/fractures into the model, after the fracture intensity has been fixed in the model generation process then how well will the chosen P_{32} be honoured by the ultimate model?
3. If the ‘complexity factor’ is applied at all scales including background fractures then what is the basic unit of generation, is it features because background fractures are made up of features?
4. The microstructural model includes such elements as the thickness of all mineral zones (i.e. intact wall rock, altered zone, cataclasite, etc) and the distance between adjacent fractures. How is consistency maintained so that some volumes of the modelled region are not assigned more than once?

It can be concluded that the resulting model is difficult to check for consistency..

5.5 Is the outcome likely to provide a successful basis for other groups?

The hydrostructural model is well defined and provides a useful test bed for Tasks 6D and 6E. The main concern with the hydrostructural model is that it is probably too well connected. This could mean that in Tasks 6D and 6E the contamination migrates so fast that it effectively doesn’t have enough time to interact with the pores and the matrix.

5.6 Terminology

The use of some terminology in the report is ambiguous and inconsistent, which makes the report difficult to understand. This was touched upon in the following requirement in the specification, namely:

"emphasise integration of information …in various reports, unification of terminology, produce clarifying figures".

To avoid such problems in the future, it is recommended that the members of the Äspö Task Force develop and use agreed definitions for 'fractures', 'features', 'structures' and possibly other terms that are commonly used in fracture flow and transport modelling.

6 References

Andersson P, Byegård J, Dershowitz B, Doe T, Hermanson J, Meier P, Tullborg E-L, Winberg A, 2002. Final report of the TRUE Block Scale project, 1. Characterisation and model development. SKB TR-02-13. Svensk Kärnbränslehantering AB.

Benabderrahmane H, Dershowitz W, Selroos J-O, Uchida M, Winberg A, 2000. Task 6: Performance Assessment Modelling Using Site Characterisation Data (PASC), November 28, 2000.

Bossart J, Hermanson J, Mazurek M, 2001. Analysis of fracture networks based on the integration of structural and hydrogeological observations on different scales. SKB TR-01-21. Svensk Kärnbränslehantering AB.

Dershowitz W, Winberg A, Hermansson J, Byegård J, Tullborg E-L, Andersson P, Mazurek M, 2003. Äspö Hard Rock Laboratory, Äspö Task Force on modelling of groundwater flow and transport of solutes, Task 6C, A semi-synthetic model of block scale conductive structures at the Äspö HRL. SKB Report IPR-03-13. Svensk Kärnbränslehantering AB.

Dershowitz B, Klise K, 2002. Evaluation of fracture network transport pathways and processes using the Channel Network approach. Äspö Hard Rock Laboratory. SKB IPR-02-34. Svensk Kärnbränslehantering AB.

Follin S, Hermanson J, 1997. A discrete fracture network model of the Äspö TBM tunnel rock mass. Äspö Hard Rock Laboratory. Progress Report. AR-97-001. Svensk Kärnbränslehantering AB.

Hermanson J, Doe T, 2000. TRUE Block Scale Project Tracer test stage. March ’00 structural and hydraulic model based on borehole data from KI0025F03. Äspö Hard Rock Laboratory. SKB IPR-00-34. Svensk Kärnbränslehantering AB.

Hermanson J, Stigsson M, Pringle A, 1999. Äspö H.R.L. – Prototype repository DFN Model No 1. Äspö Hard Rock Laboratory. SKB IPR-99-09. Svensk Kärnbränslehantering AB.

Hodgkinson DP, Black JH, 2005. Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes: Review of Tasks 6A, 6B and 6B2. Quintessa Report QRS-1178B-1, Version 1.0.

Mazurek M, Bossart P, Eliasson T, 1997. Classification and characterisation of water-conducting features at Äspö: Results of investigations on the outcrop scale. Äspö Hard Rock Laboratory. SKB ICR-97-01. (referred to by Bossart et al. 2001 as Mazurek et al. 1996). Svensk Kärnbränslehantering AB.

Poteri A, Billaux D, Dershowitz W, Gómez-Hernández J-J, Cvetkovic V, Hautojärvi A, Holton D, Medina A, Winberg A, 2002. Final report of the TRUE Block Scale project, 3: Modelling of flow and transport, SKB TR-02-15. Svensk Kärnbränslehantering AB.

Rhén I, Gustafsson G, Stanfors R, Wikberg P, 1997. Äspö HRL – Geoscientific evaluation 1997/5. Models based on site characterisation 1986–95. SKB TR 97-06. Svensk Kärnbränslehantering AB.