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How Findings from a Multi-Annual International Modeling Initiative Are Implemented in a Nuclear Waste Management Organization

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Abstract: In the present paper, we discuss various aspects of the SKB Task Force on Modeling of Groundwater Flow and Transport of Solutes (TFGWFTS). The TFGWTS is a multi-lateral forum for modeling of groundwater flow and solute transport, focusing on issues of relevance for disposal of nuclear waste. We discuss the objectives and set-up of the different tasks performed during the last 30 years, and specifically how the results of the modeling have informed performance and safety assessment applications within SKB (Swedish Nuclear Fuel and Waste Management Company, Solna, Sweden). We conclude that the TFGWFTS has been instrumental in developing modeling methodologies and tools, and in training and fostering modelers. While the early tasks were related to the construction of the Äspö Hard Rock Laboratory in Sweden and developed general modeling competence, the later tasks have served performance and safety assessment purposes in a more substantial manner.

Keywords: groundwater flow; solute transport; model comparison; model confidence

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1. Introduction

The safe disposal of nuclear waste, and specifically of spent nuclear fuel, has been recognized for a long time as key for success of the nuclear fuel cycle. Moreover, if nuclear power is to play a prominent role in the future energy mix, the disposal becomes instrumental. Central to any spent fuel repository licensing are performance and safety assessment studies of the repositories. Such applications have been performed by many countries for several decades already, but these studies typically rely on models with various degrees of uncertainties and unknowns. It has thus long been recognized that Underground Research Laboratories (URLs) play an important role in providing a test bench for repository concepts, and for performing geoscientific experiments under relevant repository conditions. Additionally, model comparison studies have been recognized as important steps toward building confidence in models used for nuclear waste applications, see, e.g., [1,2].

In this paper, we present the history, main outcomes and programmatic implications of the international modeling efforts within the Äspö/SKB Task Force on Modeling of Groundwater Flow and Transport of Solutes (TFGWFTS or simply Task Force in the sequel). Specifically, we present the different tasks that have been performed and the main results and outcomes of these tasks. Additionally, we present how these results have been implemented in the program of the Swedish Nuclear Fuel and Waste Management Company (SKB). The present paper is thus a form of review of the TFGWFTS effort, highlighting the importance of certain results and how these results have helped and improved both site-descriptive modeling and performance/safety assessment modeling within SKB. It is noted that other participating organizations may have used and implemented results in other ways; here, only the experience of SKB is provided. The motivation for not providing a unified or common experience is that the Task Force reaches a common view only on the tasks performed, not on how they should be applied. The common view is achieved through evaluation activities performed by a reviewer. How the results are to be applied in the safety assessments/safety cases of the individual organizations is not a matter of the Task Force to address, but rather an issue for each organization based on their particular natural, technical and legal conditions.

The TFGWFTS was formed in 1992 as part of the international collaboration around the newly established Äspö Hard Rock Laboratory (ÄHRL). The ÄHRL, which is located in the archipelago in the municipality of Oskarshamn in southeastern Sweden, was established as a research facility for final disposal of spent nuclear fuel. The facility was to be a test ground for geoscientific characterization methods, experiments at different scales of both the natural and engineered systems of a potential repository, and for evaluation of various deposition technologies. The ÄHRL opened up to international collaboration already from the start and based on the previous successful modeling efforts organized by the OECD/NEA in conjunction with the Stripa Project in Sweden [1], the TFGWFTS was formed. Most major nuclear waste management organizations of Europe, North America and Asia have been or are members of the TFGWFTS.

By providing the history and experiences of the TFGWFTS and showcasing how the results have been useful and important for SKB's geoscientific modeling, we argue that international modeling initiatives have been and are instrumental in gaining confidence in numerical modeling related to nuclear waste disposal. The benefits include improved models through information and experience exchange, training of personnel, a possibility to explore a greater number of conceptualizations of the same problem than single organizations and teams could achieve or afford and building of strong collegial networks. In the following sections, we first (Section 2) outline all the tasks that the TFGWFTS has addressed, and also provide some common conclusions drawn during the review process of the tasks. In Section 3 we provide the SKB-specific applications and discuss how the results and common conclusions from the tasks have served these applications. In Section 4 we provide and discuss some lessons learnt through the TFGWFTS experience. Finally, in Section 5 we summarize the main conclusions.

2. SKB Task Force GWFTS

Initially, the scope of the Task Force contained supporting, predicting and analyzing modeling studies to aid the experimental work at ÄHRL. It was realized that the predictive modeling can constitute an important corner stone in the design of an experiment, and the post-experimental analysis modeling work can provide vital components in the process understanding and interpretation of the experiment. From the beginning, the Task Force was selecting specific experiments, either planned or already performed by the ÄHRL for parallel modeling by more than one team participating in the TFGWFTS. The selection of experiments was done in consultation with the experimental projects. Later on, the scope was enlarged to be able to address relevant flow and transport experiments performed at other sites as well. Some aspects of the TFGWFTS work mode are:

- The assignments in the TFGWFTS were earlier tied to the experimental projects performed at Äspö and/or in situ data from Äspö, but now experiments from other sites as well are used.
- The goal is that the work is performed within the framework of well-defined and focused modeling tasks. Several modeling teams should preferably address each task.
- The TFGWFTS should attempt to evaluate different concepts and modeling approaches. This is achieved by several modeling teams performing the same task, followed by evaluation of the modeling work by the Task Force Delegates.
- The TFGWFTS should provide advice on experimental design to the project teams of the ÄHRL or, if desired, to the laboratory performing the experiment.
- When possible, the modeling tasks are designed to promote interaction between the experimental project teams and the modeling teams. This requires a commitment from

the modeling teams participating in a task to adhere to the project time schedule and scope.

- The modeling approach of the modeling teams complements that of the project team that is in charge of designing and executing the experiments.
- A new task can address a new experiment to be performed at ÄHRL or another underground facility in the world. It is up to the participating organizations to propose suitable experiments, and the corresponding modeling tasks. A proposed task can also address unanswered and relevant scientific questions and utilize already existing data.

Each organization participating in the TFGWFTS appoints one qualified specialist as Delegate to the Task Force. These together with the Scientific Chair of the TFGWFTS constitute the Steering Committee of the TFGWFTS. A modeling task is normally lead by one or several principal investigator(s). The principal investigators write task descriptions and provide data to the modelers. Each participating organization appoints its own modeling team(s). Often, an appointed evaluator is reviewing the work, i.e., modeling reports and how the cooperation is working within the task.

2.1. The Motivation and History of the Task Force

As mentioned above, the work within the TFGWFTS was initiated by SKB in 1992. The TFGWFTS was created to be a forum for the organizations supporting the ÄHRL project to interact in the area of conceptual and numerical modeling of groundwater flow and solute transport in fractured rock. Thereby, the Task Force could be used to support the experiments by proposing experimental designs, planning, predictions, interpretations, review and evaluation of both experiments and the modeling work. In addition, the Task Force could propose new experiments to address a scientific problem that is important for the performance and safety assessments. The experiments will in turn provide essential data for the modeling work so that the models can be used for predictions, interpretations, comparisons of results, and evaluations. Hereby, the Task Force constitutes an important platform for developments of modeling tools. Starting from Task 7, which addressed hydraulic tests performed at a site, which is now part of the ONKALO facility on the island Olkiluoto in Finland, the scope of the Task Force has widened so that the modeling work can address experiments performed at other sites than Äspö HRL. A bit later, the Task Force was renamed SKB TFGWFTS. The locations of Äspö HRL and ONKALO are shown in Figure 1.

Figure 1. The Äspö Hard Rock Laboratory (ÄHRL) is located in the archipelago near Laxemar in Sweden and the underground rock facility ONKALO is located on the island Olkiluoto in Finland (map taken from [3]).

Presently, besides SKB, the participating organizations are BMWi (Germany), DOE (USA), NUMO (Japan), NWMO (Canada), KAERI (South Korea), Posiva (Finland), SÚRAO (Czech Republic) and TPC (Taiwan). Other organizations that have been members are, e.g., ANDRA (France), CRIEPI (Japan), ENRESA (Spain), JAEA (Japan), PNC/JNC (Japan), NAGRA (Switzerland), and UK Nirex/RWM (United Kingdom). Commonly, each organization provides at least one modeling team that can be in-house, a consultant or from academia. Normally, at least one PhD student is involved in each task. More information on SKB TFGWFTS may be found at www.skb.se/taskforce (accessed on 27 December 2022).

2.2. From Task 1 to Task 10

Below, we provide a short summary of each task, and of its motivation and execution. The main results and how the results have been used in performance and safety assessment studies are discussed in Section 3. The tasks have been chosen to support the experiments performed at ÄHRL and ONKALO, for being beneficial for the participating organizations and to be useful for the model developments.

2.2.1. Task 1–LPT2 Evaluation Modeling

A large-scale field experiment, performed on the island of Äspö, was chosen as the first task. It consisted of a long-term pumping test, dilution tests as well as a series of tracer tests [4]. The experiment, which was denoted LPT2, gave an illustration of the influence of hydrodynamic dispersion on transport. The modeling work, see, e.g., [5], was later evaluated by the TFGWFTS with focus on the performance of the modeling, data collection and site characterization [6]. Thereby, the TFGWFTS supported the interpretation of the site and the experiment.

2.2.2. Task 2–Äspö Field Tracer Experiment Design Modeling

Task 2 addressed scoping, planning and design calculations for a number of planned experiments at the Äspö site on a detailed scale (1 to 10 m) and thereby it gave valuable input to planned experiments. For instance, it gave input to the planned Matrix Diffusion Experiment and the Multiple Well Experiment [7]. The outcome of Task 2 was useful for other experiments as well, e.g., TRUE-1 and LTDE-SD, which were later modeled in Task 4 and Task 9, respectively.

2.2.3. Task 3–The Äspö Tunnel Experiment (Predictive/Evaluation Modeling)

The hydraulic impact of the tunnel excavation at ÄHRL was addressed in Task 3, a modeling exercise on the 1 km scale. One of the objectives was to evaluate how the monitoring and the study of the hydraulic impact of the tunnel excavation could be beneficial for site characterization. Both predictive and inverse modeling was performed [6]. The models developed in Task 1 provided useful starting points for the predictive modeling work. In addition, Task 3 provided a good opportunity to improve modeling tools and modeling methodology.

2.2.4. Task 4–TRUE-1 Predictive Modeling

Task 4 addressed modeling of the TRUE-1 tracer tests, which were in situ experiments performed on the 1 to 10 m scale in a fracture system at Äspö HRL. The experiments contained radially converging tracer tests as well as dipole tests [8]. Both conservative and sorbing tracers were used. Later on, the experimental site was impregnated with resin and excavated [9]. The modeling exercises included supporting design calculations, blind predictions (see, e.g., [10]) and analyzing post-experimental conditions. An extensive evaluation sub-task was performed as well [11–13]. Task 4 demonstrated the influence of sorption on fracture surfaces and fracture-filling materials was demonstrated, as well as flow and transport in a heterogeneous fracture.

2.2.5. Task 5–Integration of Hydrogeology and Hydrochemistry

Task 5 addressed the integration of hydrogeological and geochemical modeling [14]. Task 5 was based on modeling of the flow of waters into the underground tunnel that forms the ÄHRL, and the chemistry of the inflowing waters, using data obtained during the construction of the ÄHRL. The specific objectives of Task 5 were:

- To assess the consistency of groundwater flow models and hydrochemical mixing-reaction models through the integration and comparison of hydraulic and hydrochemical data obtained before, during and after tunnel construction.
- To develop a procedure for integration of hydrological and hydrochemical information which could be used for assessment of potential repository sites.

In Task 5, hydrochemical data of the pre-excavation groundwater system at Äspö were used to interpret mixtures of reference waters using the Multivariate Mixing and Mass balance (M3) approach [15]. In addition, groundwater heads were analyzed to establish initial and boundary conditions for a flow model of the system. A structural model and ranges of hydraulic properties had already been established in the earlier modeling of the groundwater system at Äspö, based on investigations prior to tunnel construction. A schematic of major groundwater types used in the hydrogeochemical description is shown in Figure 2. The flow model was then used to simulate inflows into the excavation and the compositions of these inflows as well as groundwaters at various parts of the modelled domain. The simulated values would be compared with the set of observed values as a first consistency check on the model. Expert judgment and an interpolation/extrapolation tool would then be used to refine the estimates of initial and boundary chemical conditions prior to re-running the numerical models of flow and transport and re-assessing the consistency between modelled and measured values for inflows and groundwater compositions.

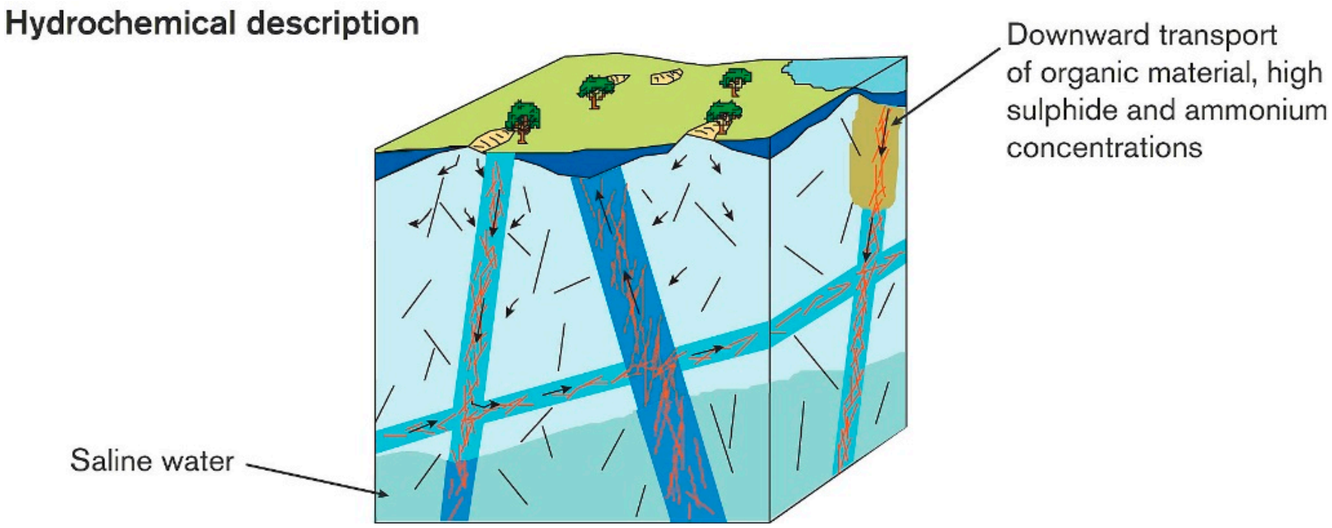

Figure 2. Schematic visualization of major groundwater types used in the hydrogeochemical description. Groundwater compositions depend on mixing and reaction processes along different recharge pathways through a crystalline rock environment consisting of deformation zones and background rock [16]. The arrows indicate the groundwater flow direction.

As mentioned, Task 5 was a hydrogeological-hydrochemical model assessment exercise, which specifically studied the impact of the ÄHRL tunnel construction on the groundwater system. Task 5 highlighted several important aspects for site investigations and facilitated the possibilities for mathematically integrated modeling and consistency checks that should be considered for future repository performance assessments. Equally important is that Task 5 has provided the opportunity to bring together two scientific disciplines that have traditionally tended to work in parallel rather than in collaboration.

There is now a much stronger appreciation that the use of hydrogeochemistry can lead to an increased understanding of hydrogeology and vice versa. Additionally, the evaluation work revealed the need for the understanding of hydrogeochemistry, development of modeling tools, and computing power [16].

2.2.6. Task 6–Performance Assessment Modeling Using Site Characterization Data

Solute transport is a key aspect of both Performance Assessments (PA) and repository Site Characterizations (SC). Focused on the 50 to 100 m scale, Task 6 provided a bridge between SC and PA approaches in fractured rock, mainly on solute transport but also on flow. This was done by applying both SC and PA models for SC boundary conditions (i.e., for tracer experiments), and also for PA boundary conditions. In summary, the objectives of Task 6 were to:

- Assess simplifications used in PA models;
- Assess the constraining power of tracer (and flow) experiments for PA models;
- Provide input for SC programs from a PA perspective;
- Understand the site-specific flow and transport behavior at different scales using SC models.

In order to fulfil these objectives, a range of modeling tasks were set-up, performed, documented in modeling reports, and subsequently evaluated. The contents of the model assignments within Task 6 can be summarized as:

- Task 6A addressed modeling and reproduction of selected TRUE-1 tracer tests using a PA model and/or a SC model to provide a common reference.
- Task 6B dealt with modeling of selected PA cases at the TRUE-1 site using relevant PA boundary conditions and temporal scales. This task served as a way to understand the differences between the use of SC-type and PA-type models, and the influence of various assumptions made for PA calculations for extrapolation in time.
- Task 6C included development of semi-synthetic hydrostructural models of fractured granite. Two scales were considered, i.e., the 200 m block and 2000 m site scale domains. The models were developed based on data from the ÄHRL experiments; the Prototype Repository, TRUE Block Scale, TRUE-1, and Fracture Characterization and Classification project (FCC).
- In Task 6D, the transport of tracers through a fracture network was modelled using the conditions of one of the TRUE Block Scale tracer tests, in the 50 to 100 m scale, and based on the semi-synthetic structural model developed in Task 6C.
- Task 6E extended the Task 6D transport calculations to a reference set of PA time scales and boundary conditions.
- Task 6F was a sensitivity study, which addressed simple test cases, individual tasks to explore processes, and tested model functionality.

Task 6 provided an improvement of modeling tools, understanding of flow and transport in DFN (Discrete Fracture Network) models, and more realistic modeling concepts to be used in safety assessment contexts [17–19] as elaborated below in Section 3. In Figure 3, an example is given of the inter-comparison of modeling results together with the corresponding field tracer test outcome.

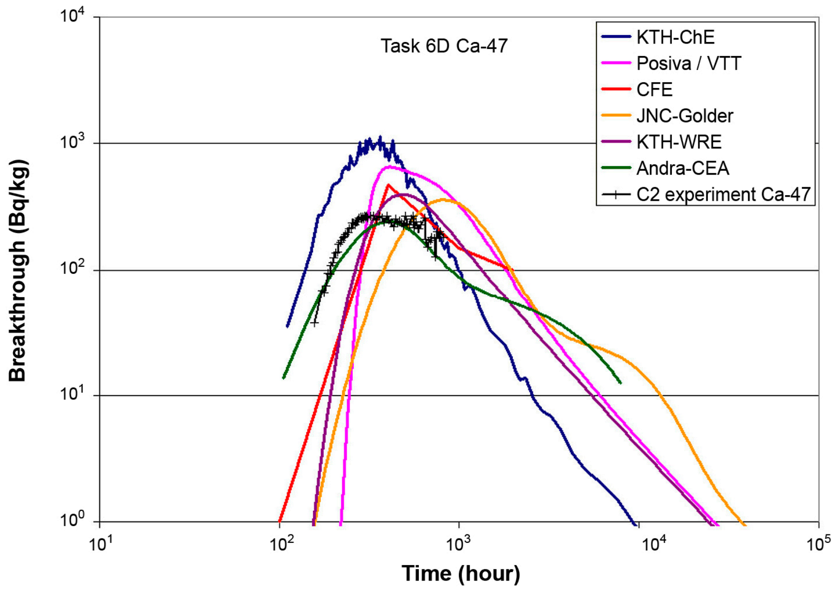

Figure 3. Inter-comparison of calculated breakthrough curves for Ca-47 in Task 6D together with the TRUE Block Scale C2 tracer test results [19].

2.2.7. Task 7–Long Term Pumping Test at Olkiluoto

Task 7 involved modeling of hydraulic tests at different scales, i.e., 1 to 1000 m, performed at Olkiluoto in Finland. Initially, a long-term pumping test performed at a scale between 100 and 1000 m was modeled. In this field test, Posiva Flow Logging (PFL) in open boreholes, and conventional pressure observations in open and packed-off boreholes were used. Task 7 addressed evaluation of the PFL measurements, but also site investigations, site characterizations, and ultimately the link to safety assessments. Usage of the PFL requires long open-hole intervals, requiring the modelers to account for the impacts of these open-hole conditions. To interpret the large-scale experiment, the focus was on increased understanding of the major fracture zones behavior as boundaries for bedrock compartments and the interaction between these "isolated" compartments and the major flow system. One example of the performed modeling work is shown in Figure 4.

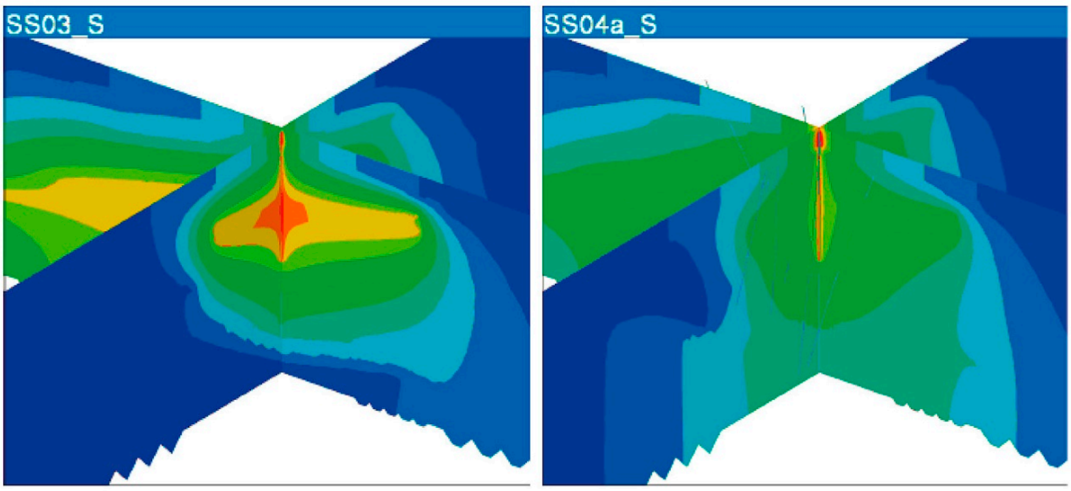

Figure 4. Contoured normalized drawdown for the Posiva/VTT small zone models for case SS03 (no monitoring boreholes) and case SS04a (including monitoring boreholes). Both are uncalibrated models (from [20]). The pumped borehole is located at the intersection of the two slices utilized for visualization purposes.

The second sub-task considered reduction of performance assessment uncertainty through block scale modeling of interference tests in five boreholes at Olkiluoto. Data were obtained from both PFL and multi-packer measurements.

The third sub-task included PFL characterization and analysis of low-permeable fractures, and assessment of flow distribution pattern at a shaft wall section at ONKALO, Olkiluoto. The PFL tests were performed in low-permeability rock at high drawdown during shaft sinking.

A feature of the modeling work was the use of PFL flow data to condition and calibrate groundwater flow models of the fractured rock. Another feature was the elements of predictive and analysis modeling. Again, the benefits of collaboration between multiple modeling teams working in parallel on a common problem using different concepts, approaches and tools were evident [20].

2.2.8. Task 8–Modeling of BRIE

Task 8 was designed to model the Bentonite Rock Interaction Experiment (BRIE), i.e., the interplay between a natural and an engineered barrier. The task was performed together with the Engineered Barrier System Task Force, and provided an increased insight of the interaction between bentonite and fractured rock at this interface of deposition holes [21]. More specifically, the objective of the task was to enhance the understanding and increase our ability to model:

- Deposition boreholes in their tunnel environment;
- Assessment of feasible deposition boreholes;
- The hydraulic interaction between the rock and partially unsaturated bentonite in a deposition borehole;
- The effects of re-saturation on the flow system;
- The understanding of post-resaturation flow and transport.

In order to obtain data for the modeling, the supporting field experiment, BRIE, at the ÄHRL was carried out. In the experiment, two boreholes, both 30 cm in diameter, were filled with unsaturated bentonite and instrumented. Thus, these boreholes may be regarded as down-scaled deposition holes. One of these surrogate deposition holes was drilled in a part of the rock domain that contained a range of water-conducting fractures. The other hole was drilled in a part of the rock domain with very few and less water conductive fractures. Total stress, pore water pressure and relative humidity (RH) were measured in the bentonite. In the rock, pore water pressure and RH were measured close to the boreholes. After suitable time, the holes were over-cored, and the bentonite analyzed mainly regarding water content distribution. In the experiment, new technologies were required to:

- Characterize the hydraulic conductivity of the rock for extremely low values;
- Characterize the dual porosity/dual permeability system;
- Monitor stress and water saturation in detail;
- Characterize the stress/pressure/permeability coupling.

The modeling task was to model the evolution in space and time of:

- In the rock: the water pressure and water flow in the rock matrix and fractures around a deposition borehole.
- In the bentonite: the water pressure, total pressure (swelling pressure), density and water content in a deposition borehole.
- At the interface: exchange of water across the interface between the bentonite and the sparsely fractured rock.

Task 8 proved to be an excellent learning exercise for both modelers normally dealing with fractured rocks and those focusing on bentonite, i.e., the interchange of information and knowledge between these communities was very fruitful [21]. Additionally, the experimentalists made advancements dealing with this challenge.

2.2.9. Task 9–Modeling of REPRO and LTDE-SD

Task 9 focused on modeling of coupled matrix diffusion and sorption in heterogeneous crystalline rock matrix at depth. This was done in the context of inverse and predictive modeling of tracer concentrations of the in situ experiments performed within LTDE-SD at the ÄHRL in Sweden, and the REPRO (Rock Matrix Retention Properties) project at the ONKALO underground rock characterization facility in Finland, focusing on sorption and diffusion. The ultimate aim was to develop models that in a more realistic way represent retardation in the natural rock matrix at depth.

The REPRO project was in part carried out in situ, and in part as an extensive laboratory program. In the in situ experiments, two water phase diffusion and sorption campaigns were carried out from the REPRO niche at about 400 m depth, from which a number of boreholes had been drilled. These campaigns were the WPDE (Water Phase Diffusion Experiment) series of experiments and the TDE experiment (Through Diffusion Experiment). The in situ part of REPRO aimed at tackling the topics of diffusion, sorption, anion exclusion, and rock matrix anisotropy. The laboratory part has, in addition, focused on small-scale rock characterization. One example of how the data were used in the modeling is shown in Figure 5.

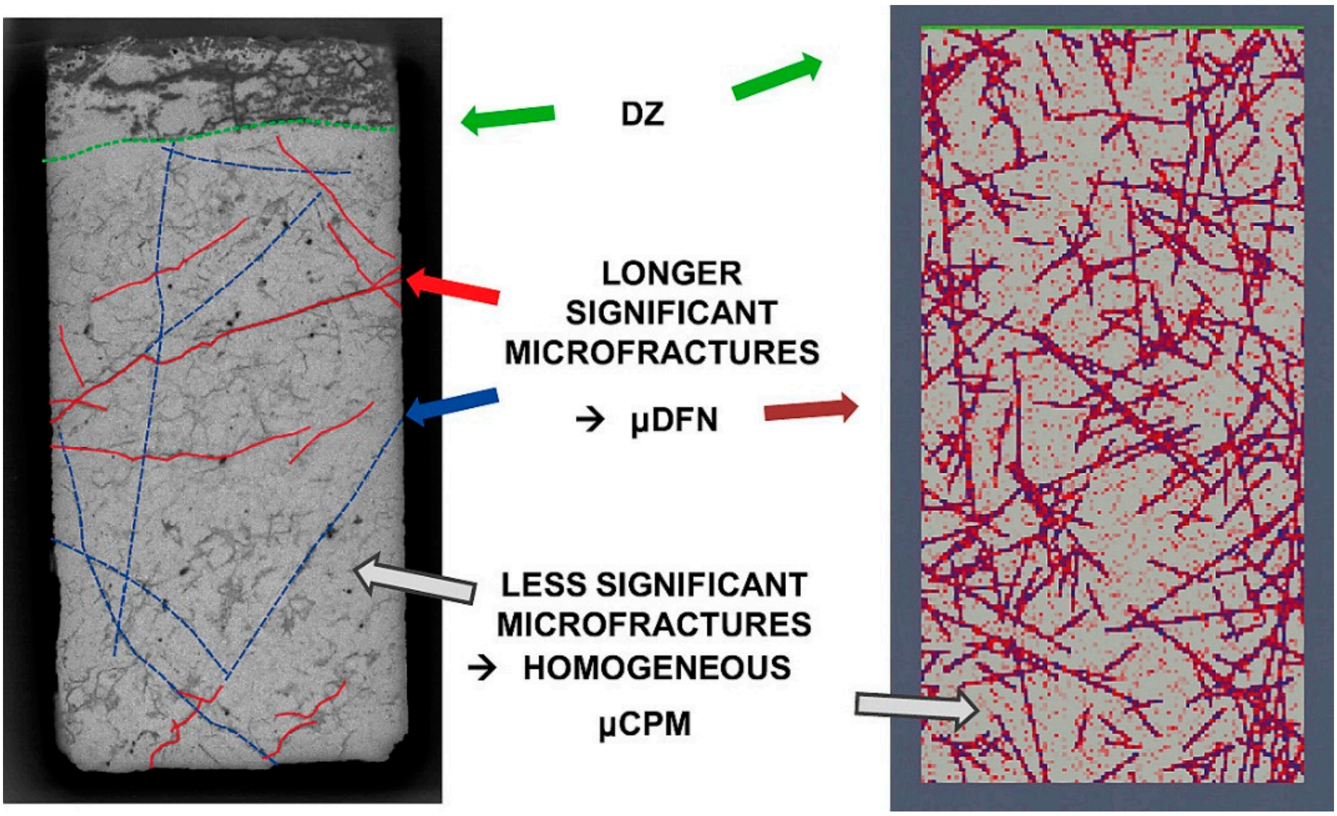

Figure 5. Definition of the basic components of the rock matrix; Disturbed Zone (DZ, which is indicated by green arrows and lines), longer significant micro-fractures, and less significant micro-fractures forming the background of the image. Rock matrix microscope photograph on the left and a micro-continuum model with a randomly generated network of micro-fractures in the cross-section on the right (after [22]).

LTDE-SD is one of only a few performed in situ studies focusing on tracer transport in the stagnant pore water of the rock matrix. In the experiment, a cocktail of both sorbing and non-sorbing tracers were allowed to contact a natural fracture surface, as well as the unaltered rock matrix, for a time period of 200 days. The experiment was carried out at a depth of about 410 m below sea level. An illustration of the LTDE-SD experimental site at the ÄHRL is shown in Figure 6.

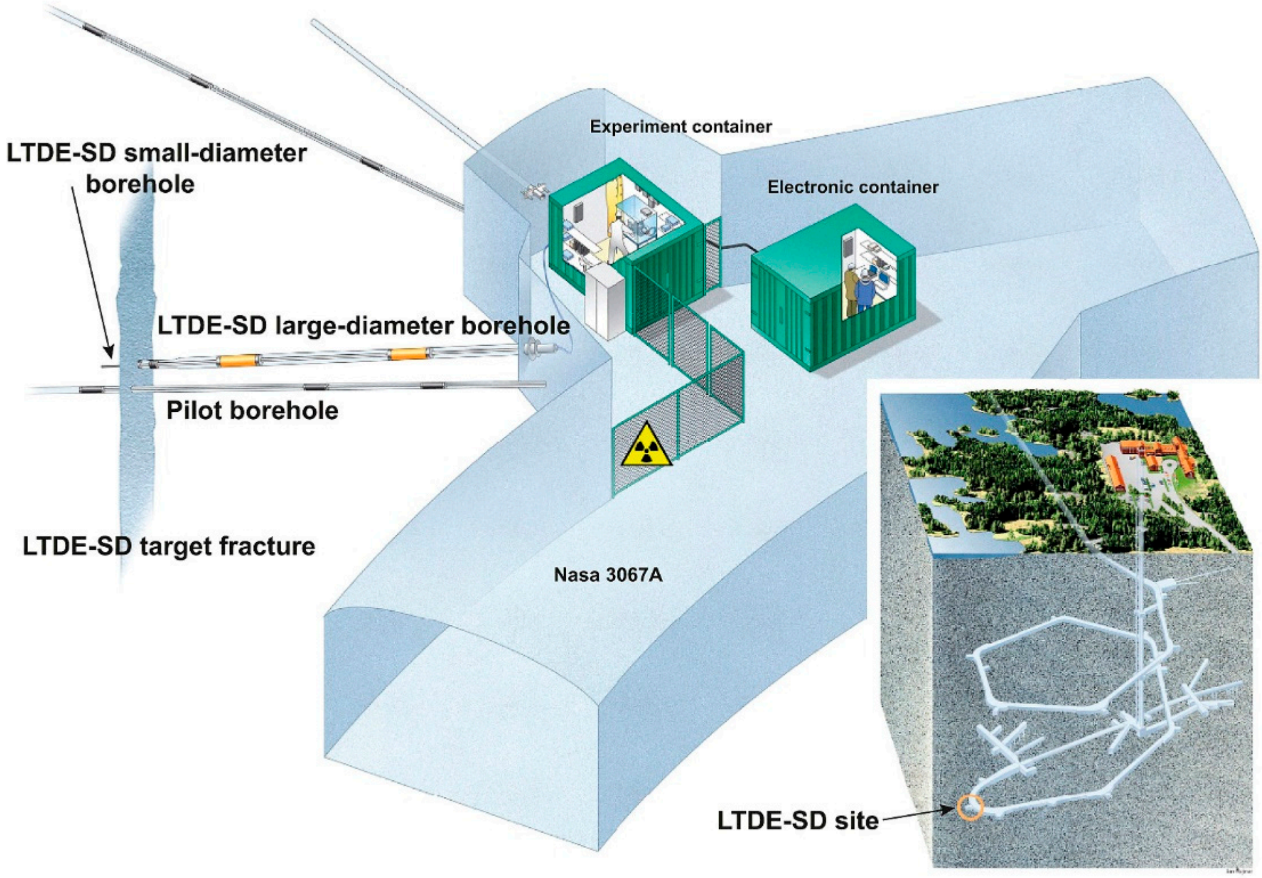

Figure 6. Illustration of the LTDE-SD experimental site at the ÄHRL, Sweden (from [23]).

Task 9 was initiated in the spring of 2015 and started with predictive modeling of the WPDE of the REPRO project [24,25]. This was designed to be a very well-defined experiment mainly addressing advection and matrix diffusion, i.e., well suited as an initial modeling task, but it proved to be a larger challenge than expected due to dispersion, both in situ and in the lab. The second sub-task focused on the inverse modeling of experimental results from the in situ tracer test LTDE-SD [22]. Eventually, the sub-task managed to explain the experimentally observed deep penetration of solutes into the rock matrix. It turned out to be an experimental artifact. In the third sub-task, the TDE (Through Diffusion Experiment) of REPRO was modeled as well [26]. This sub-task gave an excellent opportunity for predictions, model development and testing, result comparisons and evaluation. As the fourth sub-task, the increased realism in the solute transport codes was put in the perspective of safety assessment time scales. This was to highlight if different aspects of matrix diffusion and sorption, utilizing codes with increased complexity and realism, may have any consequence for long-term retardation [27].

2.2.10. Task 10–Validation Approaches for Groundwater Flow and Transport Modeling with Discrete Features

Among the objectives of the TFGWFTS are to develop, test and improve tools for conceptual understanding and simulating groundwater flow and transport of solutes in fractured rocks. The ongoing Task 10 focuses on validation of such models. Several of the participating organizations have realized and experienced that there is a need for validation and confidence building in models addressing flow and transport in discrete features. To address this topic, a pragmatic approach is chosen [28] where predictive modeling is an important tool, which is built on:

- Pragmatic validation consistent with the IAEA definition of "fit for purpose" validation considering the limited spatial and temporal scale of available characterization data. This is shown in Figure 7.
- Use of multiple conceptual and numerical models to quantify uncertainties and sensitivities due to underlying concepts, parameters and assumptions.
- Confidence building considering model conditioning, calibration and rejection. Conditioning and calibration data and methods may be particularly important where site-specific predictions are based on limited sparse data.
- Sensitivity and uncertainty assessment of key parameters.
- Progressive validation as additional data is collected, guided by the results of previous data limitations and model studies.
- Robust model audit to identify and evaluate assumptions and limitations to ensure transparency.
- Prediction-outcome exercises to evaluate whether a model is an adequate representation of the real system being modelled by comparing model predictions with in situ and laboratory observations.

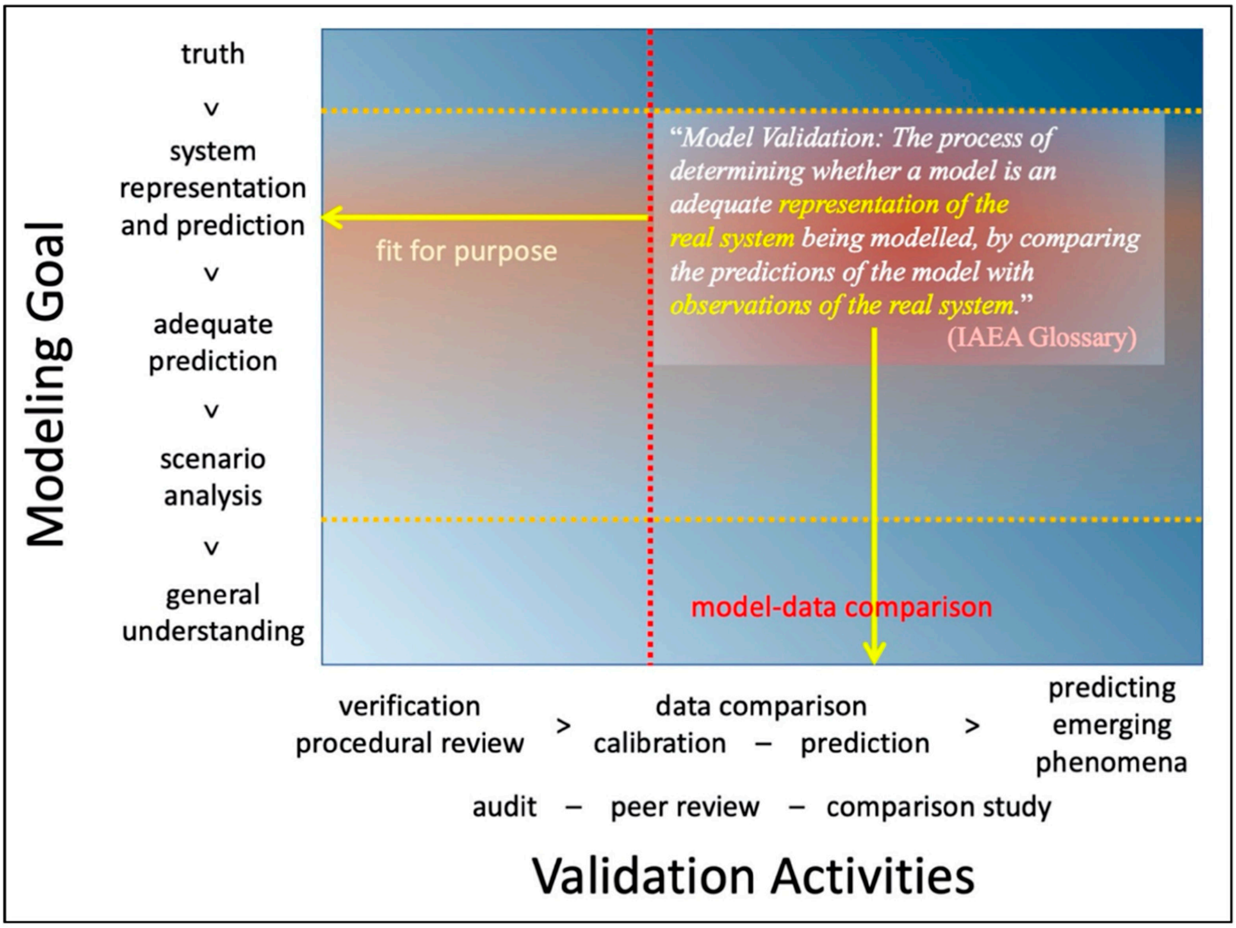

Figure 7. Approximate relation between validation activities needed to reach a particular validation goal. The yellow and red dotted lines indicate, respectively, the modeling goals and validation activities targeted by pragmatic model validation and the relation to the main goal and activity highlighted in the IAEA definition of model validation [29].

In the first validation exercises, data from granite rock blocks extracted from the Flivik quarry in the vicinity of ÄHRL are used. The objectives of these exercises are:

- Development of concepts and models for flow and transport at the single fracture scale.
- Consideration of the importance of hydro-mechanical coupling (normal loading only) on flow and transport.
- Development of modeling approaches for prediction of:
- Flow and transport in single fractures.
- Upscaled fracture properties from borehole to deposition hole scale.
- Building a starting point for pragmatic validation, i.e., a prediction-outcome exercise.

Already, Task 10 has inspired participants to publish papers, see, e.g., [30], where the water-mineral reactions in a translated single realistic fracture is addressed. In the coming sub-tasks, the same type of topics will be addressed, but for larger scales and models including networks of discrete features. For instance, in one sub-task, validation of models for flow and transport at the block scale will be dealt with. As a final exercise of Task 10, validation of models at the repository tunnel scale will be addressed.

3. Implementation in Site-Descriptive and Performance/Safety Assessment Modeling

In this section, we exemplify how the experiments listed and discussed in the previous section have contributed to modeling within site description efforts and within performance and safety assessment modeling. In the terminology of SKB, site-descriptive modeling deals with the understanding of a site's past and present conditions, while the performance and safety assessments deal with the future development. For this latter modeling, we denote the modeling of the expected behavior or performance of the repository system as Performance Assessment modeling, while the calculations aimed at quantifying radionuclide releases and associated risks for various more or less hypothetical scenarios and variants we denote as Safety Assessment modeling.

Here, we try to identify which tasks have contributed to which type of modeling, and we also try to make a judgement of the importance of the achieved results. However, first we note that the first three modeling tasks are of a slightly different nature than the other modeling tasks. This is due to several reasons; first, the early tasks were learning experiences for the Task Force, and primarily dealt with building model competence for the involved teams by predicting flow and transport responses during the characterization and construction phases of the underground facility (Tasks 1 and 3, respectively), while Task 2 was an effort to design a number of field experiments as discussed above. Thus, we do not cover these three modeling tasks in more detail but focus on the later modeling tasks. Additionally, we do not discuss the on-going Task 10 as it is premature to say exactly how the results will be used in performance and safety assessments. However, since validation of models is a key concept in any regulatory review, it is deemed certain that the results of Task 10 will be useful as a means to communicate what is achievable concerning validation in the field of nuclear waste management. The key here is the Pragmatic Validation approach [29].

3.1. Task 4

As discussed above, Task 4 dealt with modeling of transport of non-sorbing and sorbing tracers in a single feature. The main outcome of the task was the development of transport models incorporating functionality to deal with the micro-structural heterogeneity implied by a varying aperture and a matrix consisting of possibly several layers with varying diffusive (and sorptive) properties. A conceptual figure of a single fracture with an associated micro-structural model is shown in Figure 8. Additionally, the notion of the flow-related (hydrodynamic) transport resistance, e.g., [31], as a parameter governing retention in fractures was introduced and used within the TRUE-1 modeling. Additionally, it was shown how the transport resistance is an entity that is integrated along the flow paths, similar to the advective travel time. Now this concept is widely used in safety assessment studies, e.g., [32,33].

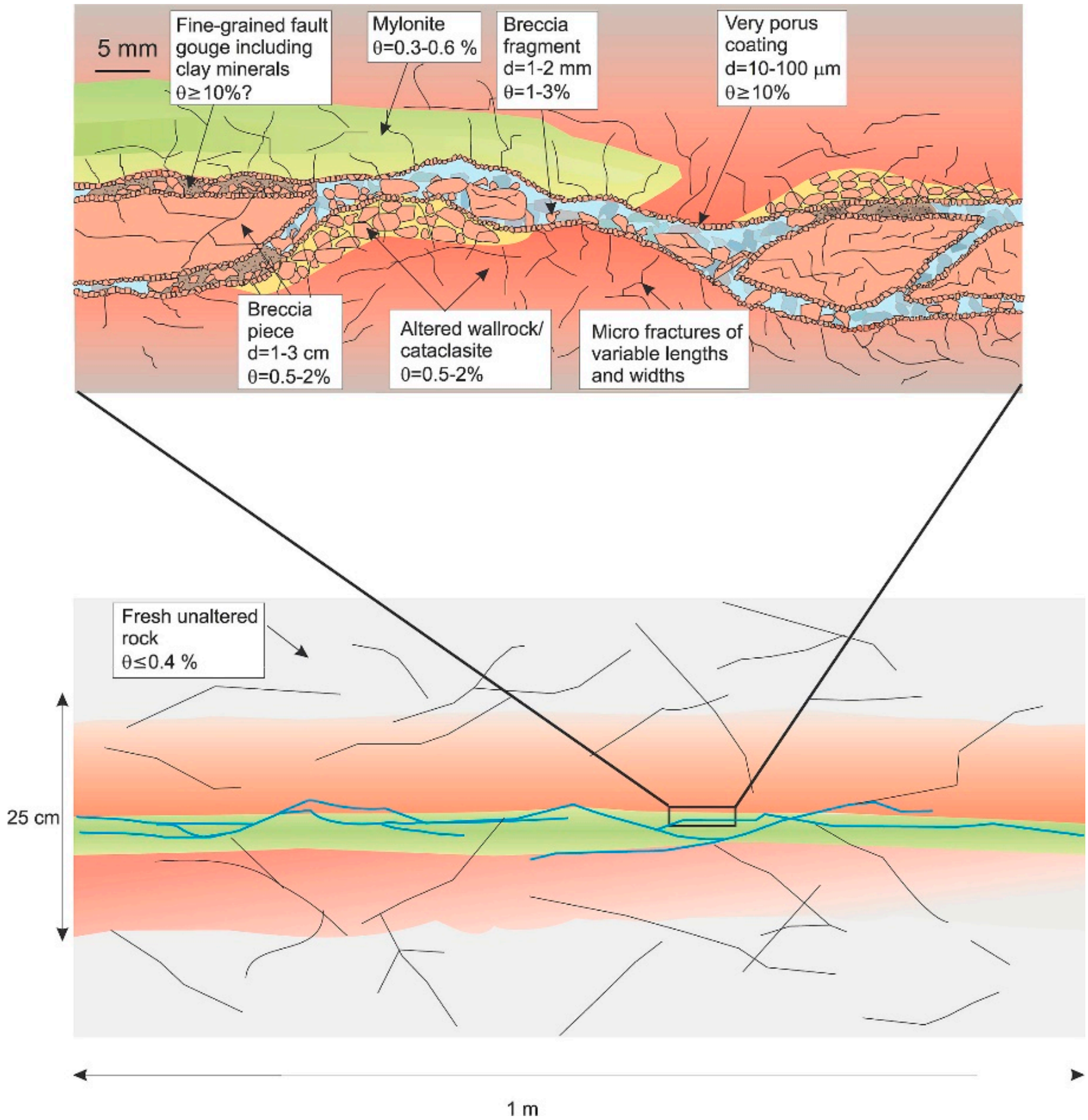

Figure 8. Conceptual figure of a single fracture with associated micro-structural model. In the figure, the symbol d represents aperture and the symbol θ porosity.

A major outcome of the TRUE-1 experiments and modeling was that diffusion and sorption data measured in the laboratory on core and crushed samples, respectively, could not be used directly to predict transport in the field. This was due to the role played by the geologic features encapsulated in the micro-structural model. Specifically, retention in possibly altered layers close to the fracture wall is stronger than that implied by the characteristics of the un-altered matrix samples. Specifically, the porosity and hence diffusivity tended to be higher in these layers. In the evaluation of Task 4 performed, the following was noted [13]:

> *"Many of the important transport and retardation parameters can only be measured in situ with great difficulty and cost. Therefore, measurements on samples in the laboratory are needed. The work within Task 4 has shown that the transfer of laboratory data on matrix diffusivity and sorption to models for field experiments is not completely*

straightforward. This is largely due to the heterogeneity in rock type along the flow path, but also due to heterogeneity within the rim zone of the fracture. These uncertainties have strong implications for the use of data in performance assessment modelling.”

While the intact rock properties farther into the matrix clearly play a significant role for non-sorbing nuclides on the safety assessment time scale, it was thus recognized by SKB that the microstructural heterogeneity may be of interest also for safety assessment applications specifically for more strongly sorbing nuclides. In the site-descriptive modeling performed for the Forsmark [34] and Laxemar [35] sites during the period 2003–2008, retardation models were formulated to capture the site-specific micro-structural characteristics [36,37]. Here, different types of fractures and deformation zones, with different retention properties, were defined and catalogued based on site characterization data. Additionally, a new radionuclide transport code for geosphere applications, MARFA, has been developed [38]. One specific key feature of MARFA is its capability to handle multiple retention models and a layered matrix. Thus, the experiences from TRUE-1 implied both a new approach to fracture characterization and parameterization, and a more sophisticated radionuclide transport model.

It is of interest to note that the experiments within TRUE-1 focused on a single geological feature, and most teams indeed modelled a single fracture or feature. However, in order to fully explain the hydraulic connections between the different boreholes, a 3D interpretation was necessary. Specifically, a discrete fracture network model implemented in FracMan/MAFIC was particularly successful in reproducing the hydraulic responses between the boreholes [13]. The use of discrete fracture network modeling also became more prominent within the SKB program after the TRUE-1 program, e.g., [39,40].

3.2. Task 5

As outlined above, Task 5 intended to use coupled hydrogeochemical models to describe the chemical evolution implied by the construction of the ÄHRL. Specifically, geochemical data prior to the construction and after construction allowed modeling the disturbance implied by the excavation. The objective of the modeling was primarily to develop tools that could handle the coupled hydrogeological and hydrogeochemical problems.

It was recognized that hydrogeological and hydrogeochemical data are used in quite different ways in such models. While hydrogeological data (such as hydraulic conductivity) or fracture data (such as transmissivity statistics) may be used to directly construct the models, hydrogeochemical data is used primarily to parameterize transport components of the model and to test whether the model can reproduce the overall geochemical evolution.

In the SKB program prior to Task 5, formal quantitative integration of hydrogeology and hydrogeochemistry had not been attempted. Groundwater flow modeling was typically done using stochastic continuum approaches including density driven flow, and hence salt transport, as needed. However, chemical reactions were not included. Quantitative hydrogeochemical modeling was primarily performed with a tool denoted M3 [41], which was based on a principal component analysis and mixing of various reference (boundary) waters. In short, any water sample could to higher or lesser degree be described as a mixing of the different components of the reference waters.

In Task 5, the perturbation induced by the tunnel construction was on a fairly short time scale, relative to a paleohydrochemical time scale, and thus mixing without reactions was rather successful in describing the geochemical change. In fact, the task was originally set up to describe how the mixing fractions developed due to the impact of the tunnel construction. However, it was noted that Task 5 was limited in understanding geochemical change on longer time scales, relevant for performance and safety assessment time scales.

However, a major outcome of Task 5 was the realization that coupled reactive hydrogeochemical modeling cannot be performed in terms of the mixing fractions of the M3 tool. Instead, to correctly model the geochemical (major chemistry) development when non-linear reactions or mineralogical heterogeneity are present, transport and chemical reactions of the individual chemical species need to be calculated. Subsequent development of coupled hydrogeochemical modeling tools within SKB's program has been based on this principle, see, e.g., [42–46]. Additionally, the use of geochemical data in hydrogeological site-descriptive modeling in order to increase confidence in modeling by showing that models are consistent between multiple geo-scientific data sets has become routine, see, e.g., [34,47].

3.3. Task 6

Task 6 dealt with bridging the gap between site-characterization and performance assessment models. The task utilized the site-characterization data from the TRUE-1 and TRUE Block Scale experiments, and thus encompassed both the singe fracture scale and block scale. The site-characterization modeling of TRUE-1 was largely similar to the earlier Task 4, but partially new teams and modeling approaches were involved in the task. The modeling of the TRUE Block Scale experiment was new to the Task Force, and here an integral part of the work was the development of a hydro-structural model of the site. While the micro-structural model of Feature A utilized in Task 4 was re-used within Task 6, an approach involving geologic structure types and complexity factors of different structures was developed as part of the hydro-structural model within Task 6.

The first objective of Task 6 was to assess the simplifications used in performance and safety assessment models, while the second objective was to determine how, and to what extent, experimental tracer and flow experiments can constrain the range of parameters used in such models.

A wide set of numerical approaches, ranging from channel network to DFN, and to stochastic continuum approaches, were adopted by the various teams. A common finding was that it was possible for all approaches to calibrate their models to the experimental transport data. However, when extrapolated to performance and safety assessment time scales, the models performed quite differently. It was also shown that when extrapolations were made, it was important to honor correlations between parameters in order to keep the prediction space as small as possible. Additionally, as in Task 4, it was concluded that the typical time scales of tracer experiments will not yield information on the properties of immobile zones, which is of main relevance for the performance and safety assessment time scales. That is, tracer tests primarily sample the near-fracture wall immobile zones, such as an altered rim zone or gouge material within the fracture. If the increased diffusive and sorptive properties of such rim zone material were to be used also on the performance and safety assessment time scales where the intact matrix becomes activated, retention would be severely overpredicted.

The findings on the Block Scale were consistent with the findings on the single fracture scale, largely indicating that retention in a network of fractures behaves as the combined effect of retention in the individual fractures. This finding is in line with what was concluded in the TRUE Block Scale project itself [48]. Assumptions on mixing at fracture intersections, however, become important at scales where multiple fractures are involved. Furthermore, the complexity factor describing differences between multiple structures on the block scale turned out to be of limited importance on safety assessment time scales, just as for the micro-structural model on the single fracture scale. Again, this was explained by the increased role of the intact rock for retention on the longer time scales.

Thus, Task 6 concluded that laboratory experiments on intact rock material are imperative for performance and safety assessment applications. However, if performance and safety assessment applications are to become less conservative, i.e., more realistic, it may be important to include the complexity implied by the small-scale single-fracture and associated matrix heterogeneity (as implemented in the micro-structural models), and the complexity factor and geologic structure type describing differences between multiple structures.

3.4. Task 7

As discussed above, Task 7 initially focused on a long-term pumping test carried out in a borehole now part of the ONKALO facility. Thereby, one initial objective of Task 7 was to simulate the pumping test in order to determine how site characterization and performance assessment can be linked, in particular by considering long-term pumping tests and measurements from borehole flow logging. Another objective of Task 7 was to better understand the effects of open boreholes on the groundwater system and to define how flow data from such boreholes could help site characterization and performance assessment. Here, it is emphasized that open monitoring boreholes were flow-logged, while the pumping (drawdown) was generated in a separate borehole.

Task 7 was successful in showing how flow-log data produced with the PFL measurement device can provide very valuable information on the flowing characteristics of individual fractures. However, the task was less successful, or rather never had the necessary time and resources, to address the link between the successful site characterization usage of flow-log data and subsequent usage of such data in performance assessment. Additionally, it was clearly shown in the modeling performed that the open boreholes constituted important connectors and pathways in the otherwise rather sparsely fractured rock. To correctly describe the hydraulic responses, it turned out instrumental to properly include the boreholes in the analyses.

In subsequent usage of the PFL tool within the SKB site characterization program, the flow logging has been performed in a slightly different way than in the experiment utilized in Task 7. Specifically, a drawdown of approximately 10 m has been imposed in each borehole in which the flow-logging is performed. By doing so, the borehole acts as a line sink, and flow along the borehole is not an issue in the interpretation (in Task 7, several pumping schemes were used, but a main setup utilized pumping in a central, open borehole, while flow logging was done in adjacent open boreholes). Thus, Task 7 served as an important inspiration for how PFL monitoring was to be performed, and how data should be used when hydraulically parameterizing a geometrical DFN model, e.g., [39]. The main features to capture in such calibrations are, in a statistical sense, the number of flowing fractures intersecting a borehole (as a subset of all fractures or all connected fractures), and their flow magnitudes.

3.5. Task 8

Task 8 was different from the other tasks of the TFGWFTS in that it was a joint task with the Engineered Barrier System (EBS) Task Force. The TFEBS has a similar role and set-up as the TFGWFTS but focuses on physical and chemical processes of relevance for the engineered barriers of the multi-barrier disposal concept. The TFEBS has specifically addressed the clay component of the engineered barriers. As outlined above, the task was based on the BRIE experiment, which dealt with water uptake in the bentonite of deposition holes located in situ in fractured rock.

The main outcome of the experiment and associated modeling was that the water uptake in the bentonite is a complex process. Specifically, the system can be categorized as either being dominated by the limited water supply from the fractured rock, or by the limited water-uptake capacity by the bentonite. This implies that the bentonite wetting is governed by the interplay between the bentonite properties and by the local fracture network characteristics, and more specifically by the discrete inflow points at the deposition hole circumference. This knowledge, and how to conceptualize and quantitatively describe it, is of course useful for the performance assessment and safety case at large. However, it also implies that if detailed saturation calculations are to be performed for individual deposition holes, local information on fracture network properties and locally conditioned models are needed. Prior to Task 8, this knowledge was not available, and clearly has implications and ramifications for performance assessment modeling strategies.

An interesting additional value of the BRIE test was that the bentonite blocks retrieved from the deposition holes clearly indicated where flowing fractures had been in contact with the bentonite. The water uptake and saturation process manifested itself through a darkening on the bentonite surface. The pictures thus produced were denoted bentographs and served as a validation metric for the modeling in the sense that individual models could be checked concerning whether they correctly reproduced the spatially heterogeneous water uptake process. A bentograph is shown in Figure 9. It should also be noted that Task 8 directly contributed to the safety case of the engineered barrier modeling by verification of the hydraulic material model for bentonite used in the THM modeling performed in SR-Site [49]. The full complexities of the water uptake process, i.e., the use of local fracture data to compute individual wetting times for each deposition hole, may only be implemented in future performance assessment studies. It should, however, be recognized that the potentially problematic holes, i.e., those with the longest wetting times, are those without flowing fractures intersecting them. Hence, water uptake in these holes is controlled by the interplay of the water supply of the intact matrix and the buffer properties.

Figure 9. Bentograph showing traces of the flowing fractures on the surface of the retrieved buffer material from a deposition hole.

3.6. Task 9

Task 9 dealt with modeling of retention, utilizing the REPRO experiments (WPDE-1 and WPDE-2) and LTDE-SD experiment. The task was sub-divided into four individual tasks as outlined above. The main findings from the first three sub-tasks, dealing with predictive and evaluation modeling of the experiments, were that a disturbed zone likely prevailed around the experimental boreholes, and that micro-structural models of the intact rock matrix were helpful in explaining some of the experimental results. These micro-structural models relaxed the assumption of a fully homogeneous matrix by introducing micro- and cm-scale fractures within the matrix, or by assuming spatially variable matrix properties. The outcome here again showed that experimental data cannot necessarily be used in, or are not necessarily relevant for, PA calculations. It should, however, be acknowledged that for the safety case it is essential to demonstrate process understanding using experimental data and detailed models.

The objective of Task 9D was then to apply the models developed in Tasks 9A-C on spatial and temporal scales relevant for performance and safety assessment applications. In this sense, the objective was similar to that of Task 6, but here the focus was on retention processes in the matrix. Specifically, the question posed was whether the small-scale heterogeneity and detail of the matrix applied in the models explaining the experimental results of Task 9A–C could be up-scaled to or abstracted on the larger spatial and temporal scales, implying in effect that such heterogeneity is averaged out on these larger scales.

The main SKB contribution within Task 9D is comprehensively summarized and elaborated in [50]. Here, reactive transport modeling accounting for micro-scale matrix heterogeneity is performed. Specifically, a description of the matrix as a micro-scale discrete fracture network with a heterogeneous distribution of sorption sites is adopted and shown to be important on small scales (such as the experimental scales of Task 9A–C) when describing solute breakthroughs of reactive tracers. Additionally, various up-scaling techniques are presented and validated at intermediate scales using independent modeling. Applying these up-scaling techniques at the scales relevant for the safety assessment of a spent nuclear fuel repository shows that the retention characteristics indeed can be captured by a very simple model using an equilibrium sorption partitioning coefficient (K_d approach) if the coefficient for the pure mineral phase is scaled to the mineral volume fraction in the matrix.

The outcome of Task 9D in fact provides a very strong argument in the quantitative safety assessment, i.e., a fairly complex model is needed to explain experimental results on the detailed scale, but the model can be abstracted and simplified on larger scales without loss of generality and accuracy.

4. Discussion

The TFGWTS has shown multiple times its usefulness in supporting the experimental work by performing scoping and design calculations, and predictive and post-experimental analysis modeling. There are several additional benefits of the activities performed in the TFGWFTS as outlined below.

An increased scientific understanding of processes important for groundwater flow and transport of solutes in fractured rock has been obtained. This knowledge is crucial for site-descriptive modeling, safety assessments and design of geological repositories for hazardous waste. While most of these processes are well-known on a general level, the modeling based on site-specific data has improved the understanding of these processes in the context of sparsely fractured rock, and specifically for applications relevant to nuclear waste disposal.

One important aspect of the TFGWFTS is the prediction of experiments and the subsequent comparison with the experimental result. Another aspect is the comparison between different modeling results, i.e., influence of conceptual models, modeling tools and/or modeling techniques [21,28]. A common scientific strategy to address conceptual uncertainty is precisely to use multiple modeling approaches, thereby increasing the conceptual model range tested. Such a strategy likely contributes to model verification and validation, and ideally leads to increased confidence in the modeling approach advocated. However, it may be practically challenging for individual nuclear waste management organizations to apply multiple modeling tools in applications and assessments. Here, the tasks performed by the Task Force may aid by providing relevant examples where multiple modeling approaches have been adopted, and hence alleviate the need for such comparisons in the programs of the individual organizations.

It is also noted that the TFGWFTS provides an international platform for sharing information and knowledge on modeling of flow and transport processes in fractured rock. While this is valuable for all participating organizations, it is especially important for organizations in early phases of their programs. Significant time savings can be achieved for a less mature organization by obtaining access to the experience and knowledge base of more advanced organizations. In addition, participation in the TFGWFTS builds and maintains scientific contact networks, while the Task Force also provides an excellent platform for development of modeling tools and methodologies, i.e., new ideas and concepts can be tested and evaluated. The work in the Task Force has traditionally resulted in several peer reviewed papers for most tasks. The experience by SKB is that studies published in the open literature greatly supports the safety case communication with relevant authorities and their reviewers. Furthermore, the tasks provide training of modelers and of PhD students. In the field of nuclear waste management-related sciences when dealing with long-term challenges is common, it is especially important to educate the next generation of modelers. Within the TFGWFTS, typically one to two PhD theses have been produced for most tasks.

The access to laboratory experimental data or data from in situ experiments performed in fractured rock at depth is key for the modeling tasks performed. Additionally, the information that is provided by the experimentalist and the principal investigators through the task descriptions is important for the value of the participation in the TFGWFTS. Access to the data and information provided by the Task Force may, to a certain extent, replace the need for nationally/locally obtained data for participating organizations. This may be especially true at early stages of a program.

In terms of task management, the cooperation between principal investigators, experimentalists, modelers, delegates, evaluators and the Task Force Secretariat has proven to be constructive. The success of a task is hugely dependent on the participants knowledge and efforts available for the given task. Additionally, a supportive and inclusive (rather than a competitive) work environment has shown to yield mutually beneficial outcomes of the tasks. In addition, a successful task execution requires competent task management in terms of high-quality task descriptions by PIs, effective task follow-up by the Task Force chairman and secretary, and informed and timely decision making by TFGWFTS delegates. In summary, benefitting from collaboration between experimentalists, modelers, principal investigators, delegates, evaluators and secretariat, i.e., the entire Task Force, the different tasks have been very useful exercises that managed to explain and interpret experimental results, develop the modeling tools further by, e.g., including more realism, improve conceptual models and demonstrate how the gained knowledge and improved tools can be used in modeling of experiments and safety assessments.

However, in addition to trying to solve scientific and technical problems, there are some challenges with the Task Force format. Work in the TFGWFTS is for most of the participants outside the regular work schedule. The TFGWFTS Secretariat has no formal control over the work of the modeling teams. However, the freedom given to the participants has stimulated creativity and proven beneficial. The participating organizations have some freedom to modify the work in the tasks to fit their needs and interests. This could of course be a benefit as well, but a challenge in the task evaluation. Often it is hard to finalize tasks as new sub-topics of interest emerge and are being pursued. The COVID-19 pandemic forced all meetings to take place online and then the time zone issue was evident for this international Task Force, which is commonly spanning 16–17 time zones. Budget restrictions require difficult prioritizations. All of the above could cause delays in reporting and finalization of the tasks.

5. Conclusions

Concerning the application of the TFGWFTS results in performance and safety assessment studies, it should be noted that the experiences discussed here are those of SKB. Other nuclear waste management organizations participating in the TFGWFTS may have reached other conclusions on how to utilize the obtained results. Some of the key take-home messages of the use of TFGWFTS results in SKB's program are the following:

- Detailed, process-based models are most often needed to explain experimental data and to defend the safety case but can often be abstracted and simplified on the scales of interest in performance and safety assessment studies.
- The TFGWFTS has been instrumental in developing and testing novel modeling approaches. This ranges from flow calibration of discrete fracture network models to description of the intact rock matrix using micro-structural models.
- Additionally, fundamental modeling concepts such as the hydrodynamic transport resistance and up-scaling of the heterogeneous intact matrix as implied by micro-structural models have been developed.

There are still a number of crucial aspects that are not addressed by the TFGWFTS, specifically a formal approach to model validation, but this is addressed in the on-going Task 10. Other outstanding issues, some already identified or new ones to be found, may be addressed in future tasks. It is concluded that the value-for-money of the TFGWFTS has been very good for SKB, and many of the most prominent modeling concepts used in the performance and safety assessment emanate from the Task Force work.

Most certainly, there will also be a continued demand for improved scientific understanding, confidence and competence building, development of modeling tools and methodologies, support for design of experiments and repositories, interpretations of experiments, safety assessments, skilled modelers, and educated delegates in the organizations. The TFGWFTS, and experimental data obtained in laboratories and underground facilities, will have an important role to play in the future.

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