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The structure of conceptual models with application to the Äspö HRL Project

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ABSTRACT (English)

In performance assessment a sequence of models is used to describe the function of the geological barrier. This report proposes a general structure and terminology for description of these models. A model description consists of the following components:

- a conceptual model which defines the geometric framework in which the problem is solved, the dimensions of the modelled volume, descriptions of the processes included in the model, and the boundary conditions,
- data which are introduced into the conceptual model, and
- a mathematical or numerical tool used to produce output data.

Contradictory to common practice in geohydrologic modelling it is proposed that the term conceptual model is restricted to define **in what way the model is constructed**, and that this is separated from any specific application of the conceptual model. Hence, the conceptual model should not include any specific data.

ABSTRACT (Swedish)

Beskrivningen av den geologiska barriärens funktion i ett slutförvar av använt kärnbränsle baseras på modellkedja. I denna rapport föreslås en generell struktur och terminologi att användas vid beskrivning av dessa modeller. En modellbeskrivning består av följande delar:

- en konceptuell modell som definierar den geometriska konfiguration som används för att lösa problemet, dimensionen på det modellerade området, beskrivning av processerna som inkluderats i modellen och randvillkoren,
- data som används för kvantifiering av storheter i den konceptuella modellen samt
- ett matematisk eller numeriskt verktyg som används för att generera resultat.

I motsats till den gängse användningen av begreppet konceptuell modell föreslås här att användningen av begreppet begränsas till beskrivning av **hur modellen är konstruerad**, och att detta skiljs från varje specifik tillämpning av den konceptuella modellen. Den konceptuella modellen skall med andra ord inte innehålla några specifika data.

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1 INTRODUCTION

The full safety assessment of a repository for spent nuclear fuel is based on a chain of models which describes the function of the natural and engineered barriers that constitute the repository concept. These models summarize the qualitative and quantitative knowledge of repository performance and are used to evaluate the future behavior of a repository. In this context it essential to recall that one of the main goals of the Äspö Hard Rock Laboratory is to

- collect material and data of importance for the safety of the deep repository and for confidence in the quality of the safety assessments.

This main goal is supplemented by the third Stage Goal for the Äspö HRL which is

- to test models for groundwater flow and radionuclide migration.

The test of models is expected to provide a basis for selecting the most appropriate models to use in the safety analysis for the licensing of a future repository.

The purpose of this report is to provide a structure for the sequence of models that have been used within the framework of the Äspö HRL Project for the purpose of describing groundwater flow and nuclide transport through the rock mass. In this context it is important to clearly define the various components of the models, what assumptions the models are based on, and how input data is provided to the models. To meet these requirements this document attempts to set up a common framework or structure for the models and to define the meaning of the terms that are used.

2 LIMITATION OF TASK

The disposal of high level radioactive waste is based on a concept that should isolate the waste from the biosphere for sufficient time to render it effectively non-toxic. Several different concepts have been developed in the countries faced with the problem of radioactive waste management. The Swedish concept for final disposal of spent nuclear fuel is based on geological disposal of copper canisters embedded in bentonite in a repository at an approximate depth of 500 m (for a general description of the concept see for example SKB-91). The safety assessment of a repository is based on a sequence of concepts of how radio-nuclides may be transported from the spent fuel rods to the biosphere and how this may cause detrimental effects to living organisms. A summary of these concepts is, for example, given in the performance assessments made by SKB (SKB-91, KBS-3).

It is not the objective of this report to try to outline the thinking and considerations underlying the overall concept of performance assessment of repositories. Instead we aim at clarifying the structure and assumptions used in defining the individual models that are used in performance assessment (in this particular case we only intend to incorporate the models applied within the Äspö HRL Project but hopefully to provide a framework that has a wider application). We will also try to show how input data are provided to each model (which normally is through use of output data from some other model) in the model sequence.

3 DEFINITION OF TERMS

A number of different physical and chemical processes influence the transport of radio-nuclides or other substances from the spent fuel to the biosphere. The processes which are judged to be of significance are included in performance assessments. These processes can be described by scientific theories.

The basic theories of physics are based on a set of fundamental principles that are held to be generally valid by the scientific community. We may term these principles as <u>basic laws of nature</u>. Examples of such basic laws are

- conservation of energy
- conservation of mass
- conservation of charge
- principles of thermodynamics
- Newton´s laws of motion

Some laws of this type are known to be approximations and are valid under a restricted set of conditions. This, for example, applies to Newton's laws of motion which are known to be an approximation valid for the velocities small relative to the speed of light that are encountered in groundwater flow problems and many other processes related to daily life.

Essentially all theories describing specific phenomena and processes are based on or have to be consistent with these basic laws. In this context we may define <u>theory</u> as a description of the principles and relationships which control a specific process or group of processes. To qualify as a theory the principles and relationships should be assumed to have general validity rather than be applicable only in specific situations. In this way a theory should provide a means for describing phenomena that occur under many different circumstances.

A model is a concept from which one can deduce effects for comparison to observations and can be seen of as an application of a theory to a specific problem (Sheriff, 1991). A 'model' may be conceptual, physical, or mathematical and can be used for

- understanding of observations and the underlying systems,
- determination of properties of a system (parameter assessment), and
- prediction of observables at other times and/or locations.

It should be noted that agreement between observations and effects derived from the model does not 'prove' that the model represents the actual situation.

In this context a model can be seen as a selection of processes under consideration and a configuration of material properties. The model may be used for the direct or *forward problem* to compute effects. Effects may also be observed and model parameters derived from the observed effects. This is termed the *inverse problem.*

In our view there is an essential distinction between a theory and a model. A theory is expected to be generally applicable while a model is used to provide a representation of a process or system for a specific purpose. Hence, a model generally attempts to describe the aspects of nature which we think are important for the problem we attempt to solve or the predictions we attempt to make. It should also be recognized that it essentially is in the definition of models that approximations are introduced. If these approximations are valid or not has to be judged in relation to the purposes of the application.

4 MODEL COMPONENTS

As described above the safety assessment of a repository comprises a sequence of models considered to represent the function of the repository system as a whole. Each sub-model in this sequence describes a process or a set of processes important for the overall performance of the system. For these models we must decide what physical processes are to be included in the model. (We have in this context assumed that chemical processes are a subset of the physical processes.) These processes should be described by some generally accepted theory. If a theory is to be quantitative is should include a mathematical description of the processes in terms of some (directly or indirectly) measurable quantities.

As stated above, a model is used to compute effects for a set of processes given some initial conditions (boundary conditions). A model can be separated into components in a hierarchical way based on the generality of the assumptions. We propose the following division:

- a conceptual model which defines the geometric (or structural) framework in which the problem is to be solved, the size of modelled volume (scale), the constitutive equations for the processes included in the model, and the boundary conditions.

- data (i.e. specific instances of the concepts) which are introduced into the conceptual model. The specific geometric representation required to solve the actual problem and the material properties are considered to be part of the data.

- a mathematical or numerical tool which is used to compute the effects (to produce output data) or to derive model parameters in case of inverse problems.

5 THE CONCEPTUAL MODEL

In order to solve a real problem we have to define boundary conditions and a geometric framework in which the problem will be solved (including the size of the modelled volume). In principle we want to find (for example) the potential $\Phi(\mathbf{r},t)$ for all values of $\mathbf{r}$ and t for a given distribution of properties, $\mathbf{P}(\mathbf{r},t)$. This cannot in the general case be done with infinite resolution, instead we have to simplify our problem so that it contains a finite number of parameters (which however may be large). This calls for a division of space into a number of geometrical units for which a finite number or parameters can be defined (normally a fairly small number for each unit). Hence, in order to solve a problem we have to provide a geometric framework or structural description of the part of nature we attempt to describe.

An assumption of structure for the material that is to be described also implies that material properties can be defined and the relationship between the fields, potentials, or the like, and the (effective) material properties. These relationships are normally referred to as constitutive equations ("equations of state" are also used in some contexts). The constitutive equations are known to represent approximations with respect to resolution (relative to material structure) and are known to have some limited range of validity. For example, Ohm's law ($\mathbf{i}=\sigma\mathbf{E}$) is not "valid" on the atomic level, and for large electrical field strengths ($\mathbf{E}$). Furthermore it is not valid for all materials. Other examples of similar relationships are Darcy's law and Hook's law. A certain constitutive equation can be used if it solves the problem under consideration with satisfactory accuracy in relation to the application.

It should be noted that the assumption of "simple" constitutive relationships like Ohm's and Darcy's laws make the differential equations linear which implies that principles like superposition and reciprocity are valid. This normally simplifies solving the equations.

Based on the set of differential equations, the material properties, and the structural description we can define a set of parameters for our model. We can then in the sense that is generally applied in inverse modelling define the output as a function of a set of parameters or in mathematical terms:

$d_i = \mathbf{F}(p_j)$ or $\mathbf{d} = \mathbf{F}(\mathbf{p})$

The parameters (p_j) will generally be of two types:

- material properties (e.g. hydraulic conductivity or transmissivity, sorption coefficients, Young's modulus)
- geometric parameters which define the structural framework (e.g. location, thickness, and extent of fracture zones, node locations of finite elements)

The output data (d_i) computed by the model are often in the form of potential or field quantities (e.g. hydraulic head, tracer concentration, stress).

In modelling we also need to define the boundary or initial conditions under which the problem is to be solved. To some extent the boundary conditions can also be considered to be parameters (p_i) that go into the computation of the output data (e.g. prescribed heads on the boundary). In other cases boundary conditions are entered as a condition on the field quantities and do not enter explicitly as a parameter in the computations (e.g. a prescribed no-flow boundary).

A major characteristic of geological systems are that they are heterogeneous with respect to the material properties. In some cases it may not even be evident how "effective" parameters should be defined. To define properties of heterogeneous media, concepts like representative elementary volume (REV) and random functions are commonly introduced. In addition, data from geologic media are generally collected in few points of the volume to be modelled and it can be debated to what extent this data is representative for other locations. This brings forth two very important aspects of geoscientific modelling. They are; 1) the *method used for assignment of material properties and geometric parameters* (interpolation and/or extrapolation) to volumes of rock where no data is available and 2) *the method used to deduce model parameters from in-situ data.* In principle, we need a model or algorithm to define the spatial assignment of parameters (material properties). This model can be very simple, for example, we can assume the medium is homogeneous and isotropic. Then there will be only one material parameter. Sophisticated stochastic models may be more appropriate in most cases. Application of such models will introduce new sets of assumptions (e.g. stationarity and ergodicity) and parameters to quantitatively describe the assumptions (e.g. standard deviations, correlation lengths, variograms). In any modelling or geologic description, the method for defining "effective" properties and assigning properties to non-measured volumes of rock should be stated explicitly.

Finally, to make quantitative predictions we need a mathematical or numerical tool (computer code, which for analytical solutions can be very simple) to generate a set of output parameters. In describing what our models produce it is important to define the output parameters. This is part of the application or realization of the model.

Above we have tried to specify what we think constitutes a model. The hierarchical structure of theories and models is schematically depicted in Figure 5-1. Below follows an attempt to more explicitly define what we mean with conceptual model and to convey our meaning of the definition by means of examples. In our opinion a conceptual model is a relatively general description or a definition of **the way the model is constructed**. This should be separated from any specific realization or application of the conceptual model. Hence a conceptual model should consist of:

- a specification of the processes (including constitutive equations) that are included in the description
- a geometric framework, i.e. a specification of **in what way** the model is divided into structural units or entities
- a specification of the parameters (both material and geometric) contained in the model
- a specification of the procedure used for the spatial assignment of material properties (parameters) to the structural units of the model
- a specification of how boundary conditions are included in the model.

The idea is that the conceptual model provides the framework for the description of nature and the framework should be distinguished from any specific realization or application of the framework. We think this is consistent with the definition of a conceptual model used by HYDROCOIN:

> "A qualitative description of a system or subsystem (e.g., important processes and interactions) and its representation (e.g., geometry, parameters, initial boundary conditions) judged to describe aspects of its behavior relevant to the intended usage of the model."

In our view, the term conceptual model is generally misused in geohydrologic modelling. The general use of the term "conceptual model" (of a site) is a description of the main features of the geology and the hydrologic importance of these features. In addition, the conceptual model is considered to provide **the** description of the site defining the exact locations of fracture zones etc. This implies that a new conceptual model is created if the location of a fracture zone is changed.

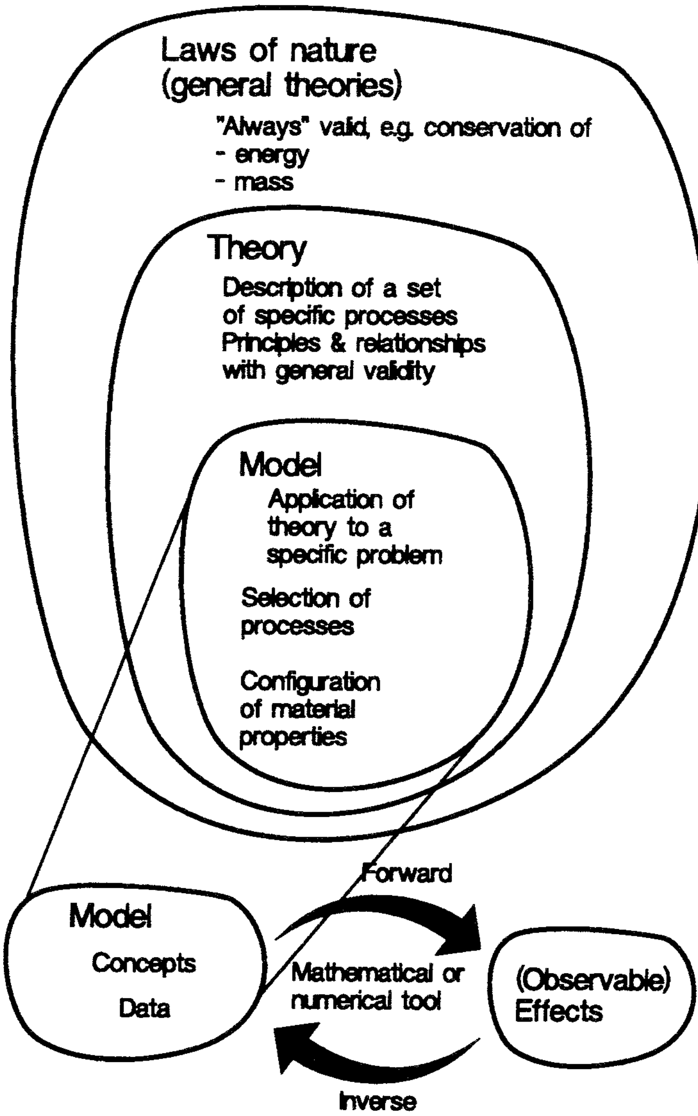

Figure 5-1 Schematic of hierarchy of theories and models.

In line with the arguments presented above, we think that a conceptual model should only define the concepts or ways of representation of nature not the actual realizations of it. For example, at Äspö we have made a model of the site based on the concept that there are (predominantly steeply dipping) fracture zones which can be distinguished from "average" rock. The model also includes the concept of rock types with different hydraulic conductivity (e.g. the fine-grained granite is more conductive).

We would like to refer to the specific description of the geology of a site (e.g. the one presented by Gustafson et al., 1991) as the "structural model" of the site. If we then, by additional investigations, get more data we can update our "structural model" and for example change the location and orientation of fracture zones somewhat. We do not think that we have changed our "concepts" if, for example, the dip of a fracture zone is changed by 10 degrees. Instead, this represents a different realization of our original concepts.

In principle the conceptual model should only include the "concept" of zones and their geometric attributes (e.g. perfectly planar but of limited extent). Their number and orientation is in this context irrelevant.

In the evaluation of the applicability (or validity) of models it is essential to be quite clear on the distinction between the concepts and the realizations because, if we are to transfer our experience to other sites, we can hope that the concepts will be transferrable but we do not expect this to be the case for specific realizations. It should be recognized that it can sometimes be difficult to distinguish between the conceptual model and its realizations. But we must try to do it!

6 THE INPUT DATA

In a model realization or application of the model, specific parameter values (including geometric parameters) are inserted into the conceptual model and a computation made to arrive at a result (effects). In this context it is important to clarify the origin of the data values that are used. The input data often come from some other model which has its own concepts, parameters, and boundary conditions. If this is the case, the model that has generated the input data should be described according to the same format as the model in which the data are used. It is evident that a sequence of model descriptions is required and that the coupling between the models has to be described appropriately.

The hierarchy of models is exemplified in Figure 6-1 which schematically illustrates how the input data to a site scale groundwater flow model is obtained from other models. The hydraulic properties that are used in a groundwater flow model are generally obtained from single or cross hole packer tests. Data from such tests (pressures and flows as a function of time) are evaluated by means of models with their own assumptions on geometric structure and material properties. The measured pressures and flows are obtained by the use of some model which describes the transducers used. The geometric data required in a site scale groundwater flow model (e.g. location of permeable fracture zones) is obtained from the structural geologic model of the site. Also this model is constructed based on input data produced by a number of different instruments each described by a model.

Site scale groundwater flow models are generally used for predictions of flow and head distributions under different boundary conditions, i.e. they are used to solve the *forward problem*. Models describing measurements or instruments are generally used to solve the *inverse problem*, i.e. to find the parameter values that best fit a given model.

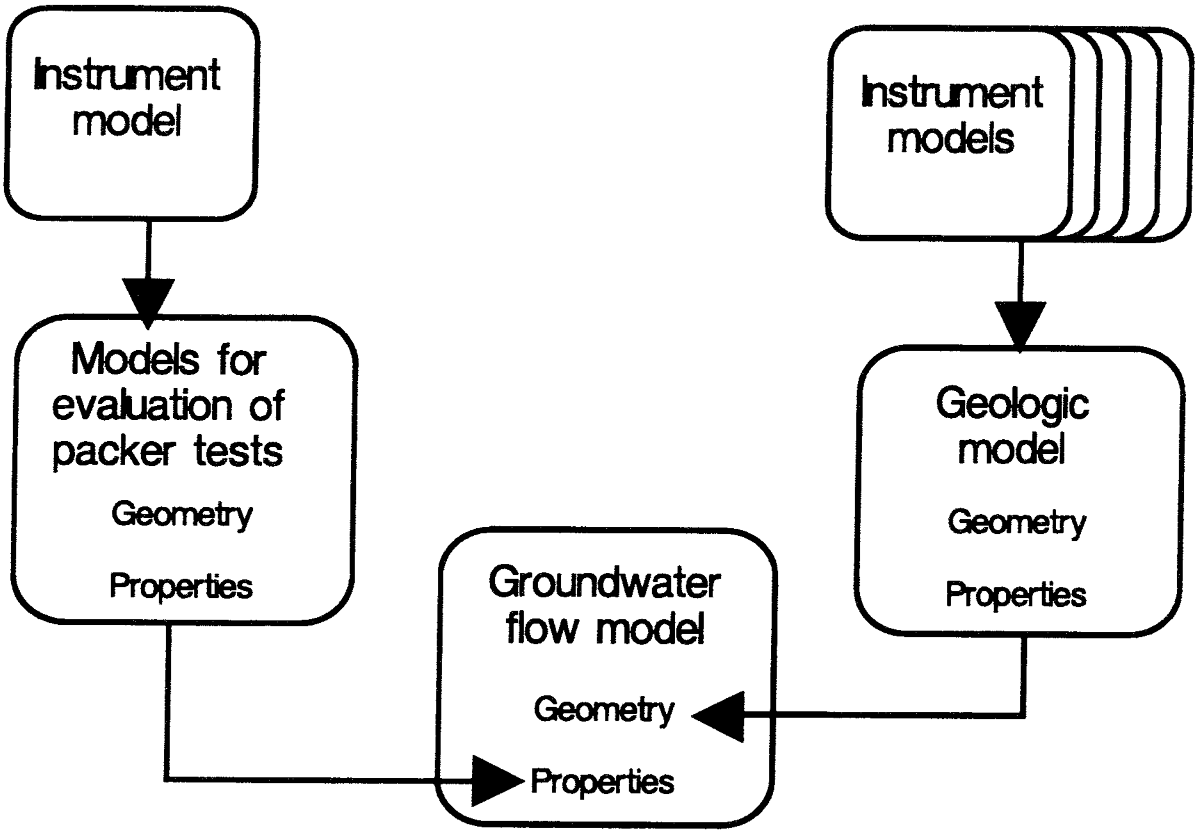

Figure 6-1 Schematic representation of how input data to a groundwater flow model is obtained from other models.

The realization or application of a model also includes the selection of a suitable mathematical or numerical tool in order to compute the output data (or effects).

7 CONDENSED MODEL DESCRIPTIONS

7.1 MODEL DESCRIPTION FORMAT

The aim is to provide condensed descriptions of the models used in the Äspö HRL Project in a common format. This should provide a means for understanding the assumptions made in modelling and how different assumptions relate to each other. A proposed format for the model descriptions is given in Table 7-1. The format is based on the arguments put forth in Section 5. An essential objective has been to condense the model description so that it would fit on a single page and still present the essential aspects of each model.

The condensed descriptions are constructed to highlight the essential aspects of each model. It is hoped that these descriptions will make the assumptions underlying each model easier to grasp and to facilitate comparison between different conceptual models.

Table 7-1 Format for condensed description of models used in the Äspö HRL Project.

MODEL NAME/DEFINITION	
Model scope or purpose Specify the intended use of the model	
Process description Specification of the processes accounted for in the model, definition of constitutive equations	
CONCEPTS	DATA
Geometric framework and parameters	
dimensionality and/or symmetry of model specification of what the geometric (structural) units of the model are and the geometric parameters (the ones fixed implicitly in the model and the variable parameters)	specify size of modelled volume specify source of data for geometric parameters (or geometric structure) specify size of units or resolution
Material properties	
specification of the material parameters contained in the model (should be possible to derive from the process and structural descriptions)	specify source of data for material parameters (should normally be derived from output of some other model)
Spatial assignment method	
specification of the principles for how material (and if applicable geometric) parameters are assigned throughout the modelled volume	specify source of data for model, material and geometric parameters as well as stochastic parameters
Boundary conditions	
specifications of (type of) boundary conditions for the modelled volume	specify source of data on boundary and initial conditions
Numerical tool Computer code used	
Output parameters Specify computed parameters and possibly derived parameters of interest	

7.2 EXAMPLES OF MODELS USED WITHIN THE ÄSPÖ HRL PROJECT

Tables 7-2 to 7-4 give condensed descriptions of the three most important models used to describe the Äspö site, i.e. the groundwater flow, the geologic, and the geochemical models. In the tables, an attempt has been made to explicitly list the parameters contained in each model, in some cases they are given within parenthesis. More comprehensive descriptions of the models are given in Gustafson et al. (1991).

The geologic model presented in Table 7-3 has a different character than the groundwater flow model presented in Table 7-2. For a geologic model it is not evident what should be meant by a process description. The geologic model describes the geometric distribution and properties of geologic features as they exist today and in principle this description does not include any physical processes. However, one of the aims in compiling the model descriptions have been to make evident the assumptions on which the models are based. From this aspect it is evident that a geologic model is based on a number of assumptions related to geologic evolution (tectonics, intrusions, erosion, glaciation, etc.) in general and the major geologic events of Southeastern Sweden in particular. Hence, we have found it appropriate to consider "geologic development" as a "process" in the description of the geologic model even though it is not as well defined and quantitative as the process of Darcian flow used in the groundwater flow model. It should also be noted that the process of arriving at the geologic model from the input data (observations) is not straight forward. It is a process which to a large extent involves expert judgement and the numerical tools are in this case used to assist interpretation rather than to compute "effects" directly from input data.

Table 7-4 reflects the fact that several different approaches for spatial assignment of properties and hence numerical codes have been used within the geochemical modelling program for the Äspö HRL. The approaches used are described by Wikberg et al. (1993).

Table 7-2 Condensed description of the groundwater flow model of the Äspö site used within the Äspö HRL Project.

GROUNDWATER FLOW MODEL OF ÄSPÖ SITE Stochastic continuum model	
Scope: natural flow, flow to laboratory tunnel, cross-hole tests (calibration)	
Process description Continuity equation (mass rate) Equation of motion (Darcy's law including density driven flow)	
CONCEPTS	DATA
Geometric framework and parameters	
3D box divided into: 2D fracture zones, planar with limited extent (location, orientation, size) Rock Mass Units (location of boundaries) Subvolumes (cells) between fracture zones	Size: 1.9x1.5x1.3 km Zone geometry from geologic model (descriptions basis for selection of "important zones") Regular grid of 20 m cubes Spatial distribution of 5 rock mass units (RMU) with 50 m thick slabs (with depth)
Material properties	
Zones: Transmissivity (T_i) Subvolumes: Hydraulic conductivity, isotropic (K_j) Salinity field	T and K from hydraulic borehole testing Salinity measurements in boreholes
Spatial assignment method	
Transmissivity: Deterministic assignment Hydraulic conductivity of cells: log-normal distribution based on RMU, depth. K and σ dependent on cell size	Transmissivity: single- and cross-hole testing Stochastic distribution of K from borehole testing
Boundary conditions	
Upper: fixed infiltration rate on Äspö, constant head at sea and peat areas Lower: no flow Side: prescribed pressure (hydrostatic) Salinity: prescribed initial conditions, linear increase with depth Tunnel: skin for rock and zones, prescribed pressure (atmospheric)	Infiltration data Salinity of Baltic Sea, salinity measurements in boreholes
Numerical tool PHOENICS	
Output parameters Pressure, density (derived parameters: flux, salinity)	

Table 7-3 Condensed description of the geologic model of the Äspö site used within the Äspö HRL Project.

<table>
<tr><td colspan="2">GEOLOGIC MODEL OF THE ÄSPÖ SITE</td></tr>
<tr><td colspan="2">Scope:
Description of lithology and tectonic structure, site scale</td></tr>
<tr><td colspan="2">Process description
Geologic development of SE Sweden in terms of tectonization, post- and macrogenic intrusives, faulting, and fracturing.</td></tr>
<tr><td>CONCEPTS</td><td>DATA</td></tr>
<tr><td colspan="2">Geometric framework and parameters</td></tr>
<tr><td>3D box with
Lithology: Granitic rocks with lenses and xenoliths of minor rock types (summarized location of units)
Fracture zones: Essentially sub-vertical dip, possibly also some low-dipping. (location, orientation, width)</td><td>Size: 2x2x0.5 km
Coordinates for fracture zones and lithological sub-volumes based on interpretation of remote sensing, surface, and borehole measurements</td></tr>
<tr><td colspan="2">Material properties</td></tr>
<tr><td>Lithology: fracture density, composition (descriptive)
Zones: character (tensional/shear, classification; major/minor, fracturing)</td><td>Geophysical data, core mapping data, rock mechanical data at observation points, thin sections, chemical analyzes</td></tr>
<tr><td colspan="2">Spatial assignment method</td></tr>
<tr><td>Lithology: averaging, probabilistic with trends
Fracture zones: deterministic (probability classification)</td><td></td></tr>
<tr><td colspan="2">Boundary conditions</td></tr>
<tr><td></td><td></td></tr>
<tr><td colspan="2">Numerical tool
CAD system
Model for interpretation of input data on fracture zones and lithological volumes at observation points</td></tr>
<tr><td colspan="2">Output parameters
Location and character of fracture zones.
Rock type distribution in previously unknown areas.
(Subvolumes with probabilistic lithology description.)</td></tr>
</table>

Table 7-4 Condensed description of the geochemical model of the Äspö site used within the Äspö HRL Project.

GEOCHEMICAL MODEL OF THE ÄSPÖ SITE	
Scope: Groundwater composition in fracture zones	
Process description Mixing of water with different composition Calcite saturation pH and Eh relationships Groundwater-rock interaction	
CONCEPTS	DATA
Geometric framework and parameters	
Homogeneous medium (3D) within permeable zones (location)	Size: 2x2x0.5 km Zone locations (from geologic model) to determine valid output locations
Material properties	
Concentrations of Na, Ca, K, Mg, Cl, SO_4, HCO_3, Fe, HS pH, Eh	Groundwater sampling in boreholes and in the sea
Spatial assignment method	
Principal component analysis (correlation) Linear regression, Neural networks, Kriging	pH, Eh, and ion concentrations at sampling points, location of sampling points
Boundary conditions	
Composition of groundwater used in mixing calculations (end members) (obtained from constitutive equations) Salinity at the boundary of the groundwater flow model	Calculated end member composition (inverse modelling) Salinity at the boundary of the groundwater flow model as a function of depth
Numerical tool	
PARVUS, Brainmaker, Statistica, Statgraphics, Surfer Expert judgement	
Output parameters	
Groundwater composition at selected points (within zones) prior to and after excavation of laboratory tunnel (steady state conditions)	

8 CONCLUSIONS

We consider the proposed format for condensed model description provides a means for presenting the essential aspects of models used in performance assessment. The examples presented above has been a first attempt at applying the proposed format. The intention is to continue the work and apply it to other models that have been used within the Äspö HRL Project. It is anticipated that this work will provide deepened insight into the usefulness of the proposed format and that minor modifications will be motivated.

In this work we have proposed a definition of the term conceptual model which is slightly different from the general use in geohydrologic modelling. We proposed that the term conceptual model should define **in what way the model is constructed**, and that this should be separated from any specific application of the conceptual model. Hence, the conceptual model should not include any specific data.

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[1] Vibrometric Oy, Helsinki, Finland
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[1] AECL, Canada
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[1] Department of Geology, Chalmers University of Technology/Göteborg University
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Peter Andersson (ed.)[1], Anders Winberg (ed.)[2]
[1] GEOSIGMA, Uppsala, Sweden
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