Groundwater Chemistry in SKB's Safety Assessment SR-Site

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Scope of reports and approach to review

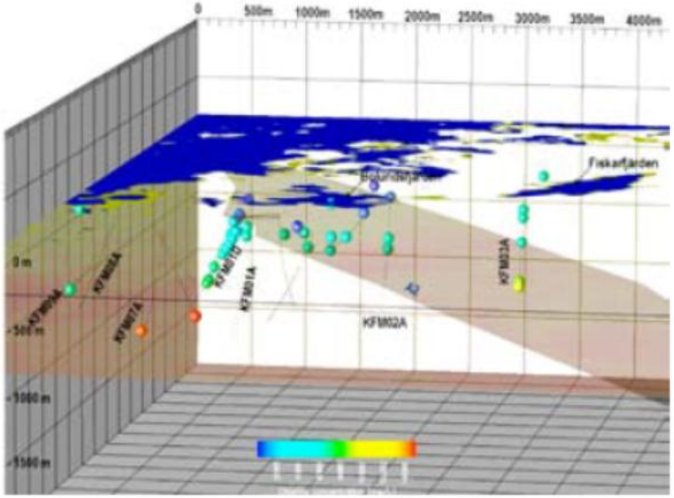
- Main SR-Site reports
  - TR-11-01 Main Report (Vols 1, 2, 3)
  - TR-10-52 Data Report
  - TR-10-48 Geosphere Processes
  - TR-08-05 Site Description, SDM-Site
- Hydrogeochemical reports
  - TR-10-58 Hydrogeochemical Evolution
  - TR-10-39 Sulphide Content in Groundwater
  - TR-10-57 Oxygen Ingress in the Rock
  - [R reports for SDM-Site]
- My approach to this review
  - Clarity and transparency for target readers
  - Scientific robustness in wider context of geochemistry and hydrogeology
  - Data traceable from site description through interpretation & models
  - Propagation of data/parameter uncertainties & alternative conceptual models
  - Focus and substance in relation to safety-relevance and site understanding

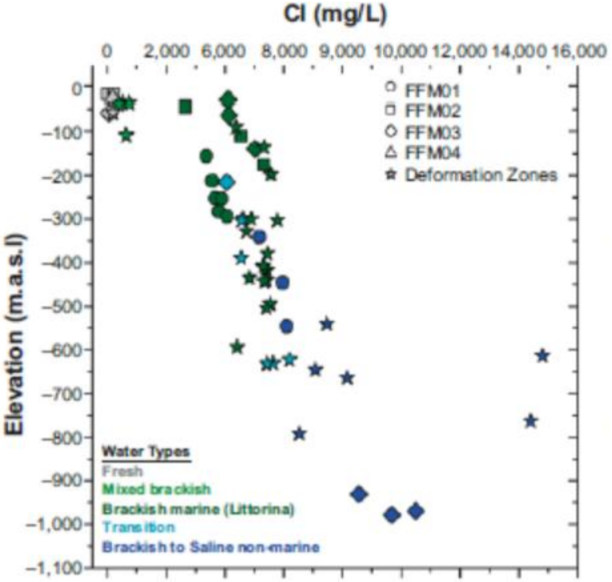
General impressions and comments

- Well written & illustrated narrative but lacking coherent quantification of site properties, interpretations and parameters (these may be in supporting reports);
- Difficult to follow how site characteristics, especially ones that indicate spatial heterogeneity and complex evolution, are represented by the choices of safety assessment model parameters;
- Focus of interpretation and detail of modelling, in some parts, is disproportionate to the scope and safety-relevance;
- Rationale for choice and scope of some interpretative models, and significance of the outcomes, is not always discussed;
- Research studies are reported that sometimes are inconclusive or inadequate for understanding the system and constraining the processes;
- Scientific robustness of interpretations is sometimes weak, lacking support from the wider literature to support SKB and site-specific research.

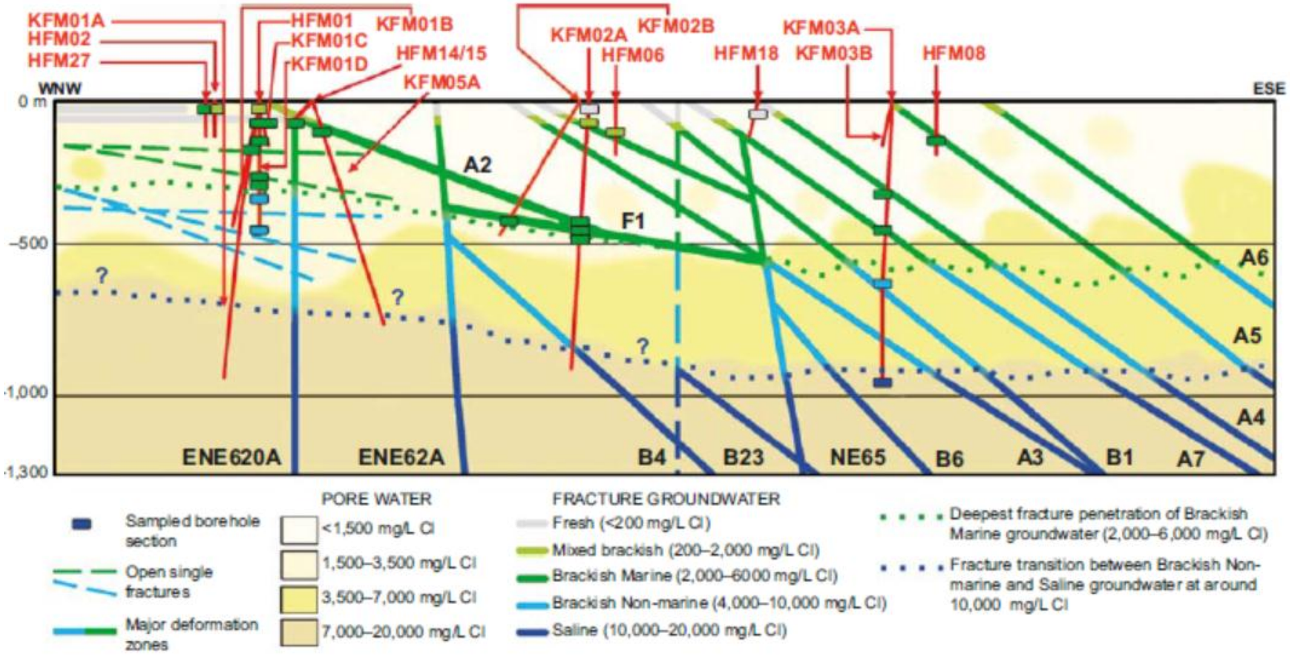
Data sources for groundwater chemistry

- ‘Key’ hydrochemical and isotopic data should be in SDM appendices (full spreadsheets have been obtained from SKB);
- Reliability of samples and analyses is mostly what is reasonably achievable;
- Some data are problematic, e.g. dissolved O_2, microbes, trace elements;
- Sparse sample distribution, especially at >600m and in NW of target volume, so alternative interpretations of heterogeneity;
- Anomalies and outliers need better consideration in SDM.





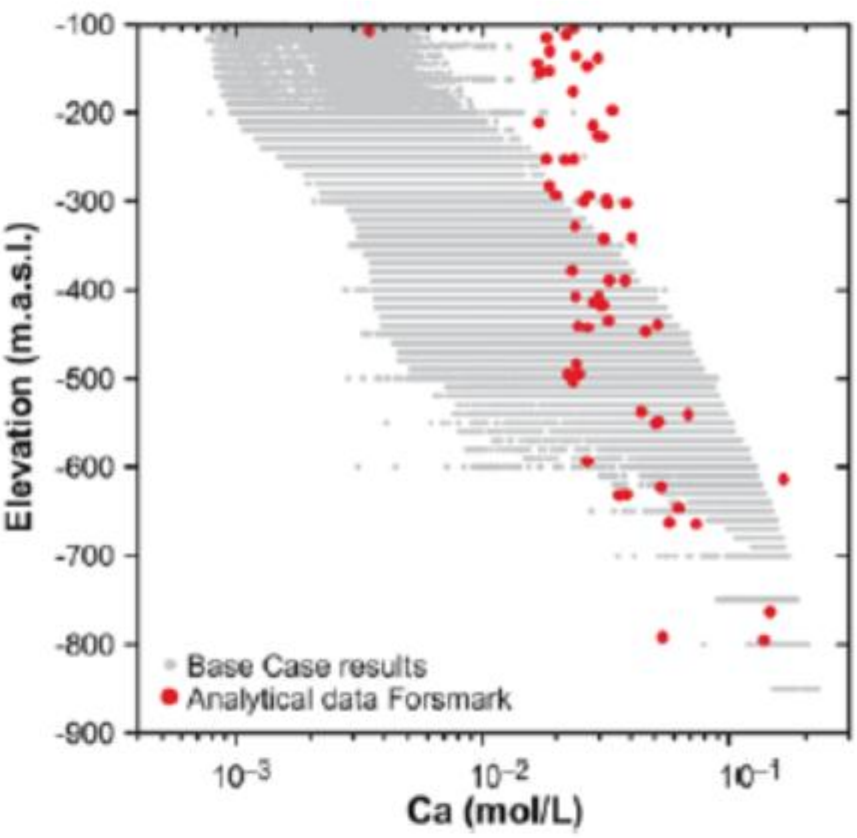
Description of initial state



- Hydrochemical heterogeneity should be interpreted and integrated with groundwater model, e.g. in terms of palaeohydrogeology, compartmentalisation of properties, and other alternative models;
- Compositions of porewaters in rock matrix and their significance for long-term evolution and matrix diffusion is an open issue;
- Interpretation of water-rock reactions is too simplistic as a basis for modelling of future evolution of groundwater compositions.

Conceptual models for hydrogeochemical processes

- ‘Allows description of geochemical heterogeneity by loose coupling’ – mixing ± reactions?
- Cation exchange (‘insignificant’ because of high salinity) and silicate minerals are omitted – modelled M^+ & M^{2+} are not realistic (figure);
- Chemical evolution models have various simplifications and may not represent full variability for safety function indicators;



Handling of uncertainties in data and processes

- Largest uncertainties in knowledge of safety-relevant groundwater chemistry at any point in reference evolution are:
  - redox conditions, Fe, HS^- and microbial populations
  - Mg, K, Ca & Na
  - Ionic strength (especially at >600m)
  - Uranium and analogue trace elements
  - Compositions of pore waters and other less mobile groundwaters in fracture domain bedrock.

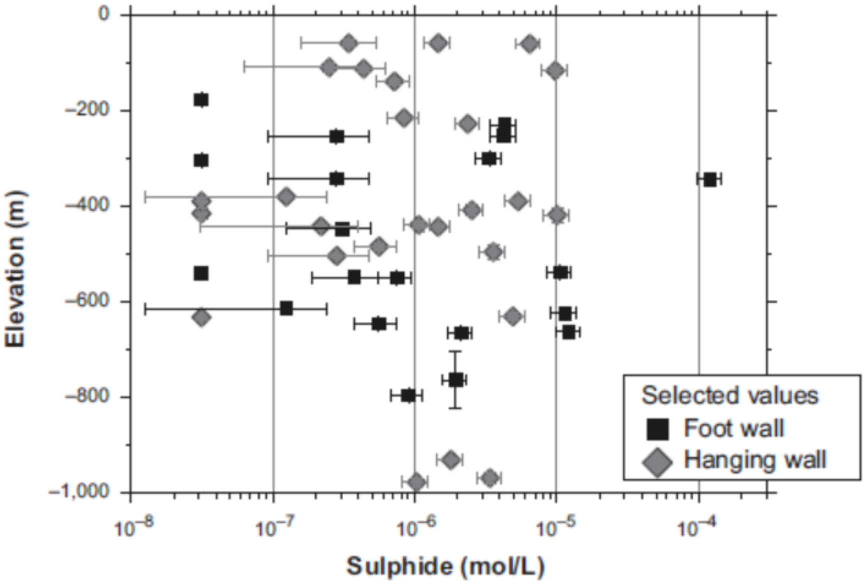
- Largest uncertainties in hydrogeochemical processes are:
  - Biogeochemical reactions causing HS^- production and controlling maximum concentrations
  - Fe mineral sources for water-rock reactions buffering redox and dissolved Fe
  - Fracture minerals and matrix controls on cation exchange and other processes affecting retardation of radionuclides.

Safety functions and groundwater chemistry

Six safety functions indicators (R1a to R1f) refer to groundwater chemistry

- What are the uncertainties on the quantitative criteria?
- Two have unquantified criteria ('reducing' as a proxy for zero dissolved O_2; occurrence of Fe, HS^- and microbial populations); how are these applied?
- M^{2+}/M^+ criterion for colloid stability is simplified to ionic strength; will this always be valid for assessing colloid stability?

Near-field geochemical and microbial processes



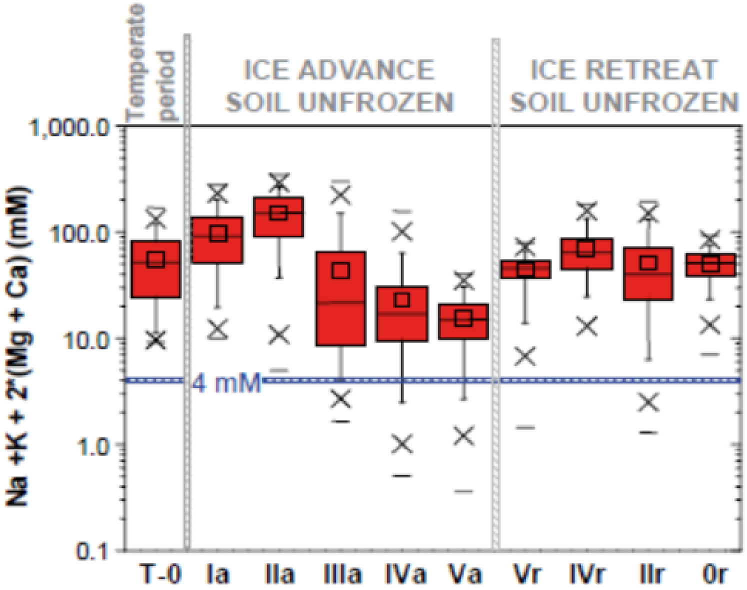
- More information is needed on whether a biogeochemical model is used to scope dependence on microbial populations, introduced materials (e.g. raised NO_3 in Äspö inflows, organics) and to constrain HS^- concentrations;

- Perturbations due to construction are scoped (e.g. persisting alkaline plume, pH ≤9) but effects on lowering of Ca^{2-} and on bedrock properties may be neglected;
- More information needed on potential range of variation of near-field groundwater chemistry at different stages of reference scenario, e.g.
  - dilute water influx in temperate climate state, global warming variant and glacial state
  - heterogeneity of water compositions in bedrock around deposition holes

Long-term evolution of groundwater chemistry

Three generic climate states plus global warming variant;

- Temperate period (& global warming variant):
  - 40m uplift – integration with groundwater modelling
  - why is it modelled only to 7000y (note global warming variant to 60000y)?
  - uncertainties in the groundwater condition at repository depth need to be clarified, noting that modelling uses only single meteoric end-member composition.
- Periglacial period:
  - clarification of uncertainties in amounts and compositions of water flow at repository depth
  - conceptual models and evidence from mentioned study sites and from 2D model should be evaluated critically, plus hydrochemical variables (DOC, SO_4, CH_4)



- Glacial period:
  - Sub-glacial hydrodynamic models, scenarios and durations represent a limited range of possibilities
  - Range of chemical variations in melt water and of geochemical evolution is narrow with ‘large degree of uncertainty’

Integration with hydrogeology and solute transport

- SKB’s palaeohydrogeology model is calibrated with salinity and mixing proportions of ‘end-member’ water compositions
  - Are alternative initial and boundary conditions, e.g. salinity at base of model, and model durations taken into account in uncertainties?
  - Is the calibrated physical hydrogeology model consistent with hydraulic properties?
  - How is the calibrated groundwater and solute transport model translated into the radionuclide transport model?
- Shallow bedrock ‘aquifer’ and bedrock to ~150m depth
  - Does the model for hydrogeoiogy, water compositions and future evolution need more data and interpretation?
- Significance of matrix pore water compositions and variability remains an open issue
  - Data may have unrecognised sources of error
  - Varying salinities in connected pores may have hydraulic implications
  - Is the distribution of compositions with respect to conductive fractures consistent with matrix diffusion?
  - Are there implications for hydrogeology of fracture networks within fracture domains bedrock units?

Hydrogeochemistry of radionuclide analogues

- Distribution of dissolved and sorbed radionuclide analogue elements (e.g. U, Ra, I, Ni, REEs, Se, Cs) in groundwaters and reactive minerals is of potential interest;
- SKB has measured most of these and has concluded that trace element data in groundwaters are uninterpretable (or too close to analytical detection);
- Anomalous U concentrations occur in some groundwaters and have been interpreted as having a local origin;
- What might be learned, if anything, about long-term retention processes from more detailed studies?