

Initial Review of Groundwater Chemistry in SR-Site

Jude McMurry and Paul Bertetti
Center for Nuclear Waste Regulatory Analyses
Southwest Research Institute®
San Antonio, USA

Outline

- Objectives and Approach
- Topics examined broadly by the initial review
 - SKB groundwater data acquisition process
 - Paleohydrology model
 - SKB approach to estimating future conditions
- Initial review findings
- Requests for supplemental information
- Additional comments and questions

Objectives and Approach

- Assess the clarity, comprehensiveness, and traceability of the groundwater chemistry information used to support the site safety case
 - Are the SKB data reasonable and sufficient to characterize the existing geochemical conditions at the Forsmark site?
 - Comparison of conceptual models, hydrochemical model output, field data
 - Trace original data from collection to model use
 - Are the methods utilized by SKB appropriate and sufficient to define the geochemical evolution of groundwater that will interact with the near-field environment over long time periods?
 - Examine use of geochemical modelling
 - Examine use of reasoned arguments
- Identify topics that require a more detailed review

SKB acquisition and use of groundwater data

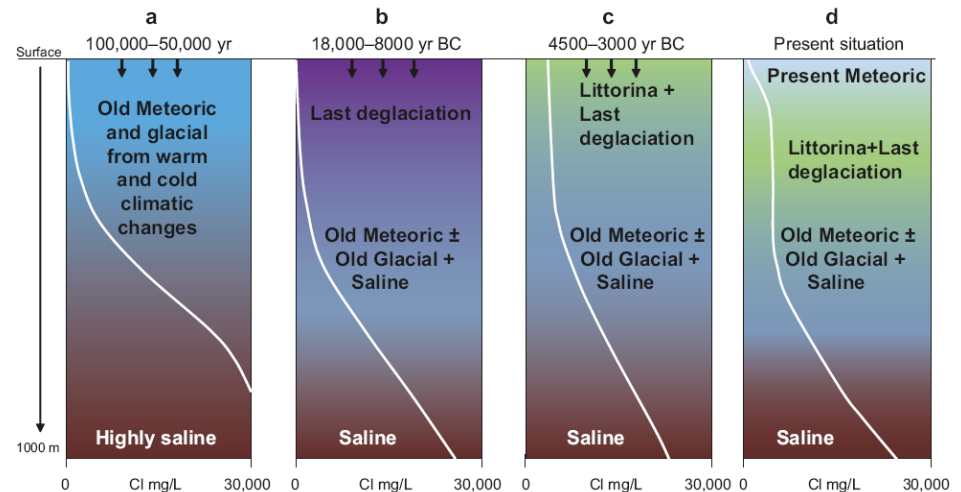
- SKB implemented an integrated hydrochemical characterization process, with a detailed suite of chemical and isotopic analyses
 - Cored borehole, percussion boreholes, surface/shallow sampling, Complete Chemical Characterisation (CCC), monitoring wells
 - A limited amount of “better” (Category 1-3) data
 - A limited use of field results to verify modeling efforts
- Interpretations of data were iterative
 - Conceptual models were revised as more data were accumulated
- Data were used primarily as input to conceptual models and detailed interpretations
 - Support for reasoned arguments
 - Sulphide concentrations
 - Reference end-member water compositions

SKB paleohydrology model

- Conceptual groundwater chemistry model included structural features and density controls on groundwater movement and composition
- Used a statistical approach, Principal Component Analysis (PCA), to identify 5 end-member water compositions at the Forsmark site
- Used site data and PCA to develop a paleohydrology model to account for the evolution of groundwater chemistry during the last glaciation

SKB conceptual model for the past evolution of Forsmark groundwaters (including the five representative end-members), from before the last previous glaciation through present-day conditions

(Figure 2-19 from Laaksoharju, et al., 2008, SKB Report R-08-47)



SKB approach to estimating future geochemical conditions

- Evaluated three distinct periods, using different approaches for each
 - Excavation and operational period (~100 years)
 - Short-term geochemical changes related to drawdown, upwelling, ventilation, repository materials
 - Temperate climate (~10,000 years)
 - Groundwater flow model (Joyce, et al.) mixing 5 end-member waters
 - Geochemical modelling of mixing and mineral equilibration (PHREEQC)
 - Glacial cycle climates (~100,000 years)
 - Groundwater flow models (Vidstrand, et al.) mixing 2-3 end-member waters
 - Geochemical modelling of mixing and mineral equilibration (PHREEQC)
 - Dynamic changes in water chemistry (recharge, upwelling, submergence, permafrost)
- Used geochemical modelling results to address geochemical safety functions
- Used reasoned arguments to address uncertainties about some future concentrations (e.g., sulphide)

Review findings: Site data and paleohydrology

- Hydrochemical characterization appears to be sufficient
 - Strong points: Collection documentation, descriptions of interpretive analyses
 - Weak points: Difficult to track exactly which data are used in some model components
- SKB identified sulphide concentrations as an important but uncertain contributor to a safety function and (appropriately) dedicated additional effort to screening and improving the usefulness of the collected data (i.e., TR-10-39)
- SKB provided little or no Forsmark data for the increasingly saline water that is predicted to occur at depth (basis for an end-member water)
- SKB's paleohydrology model is reasonably complete
 - Used detailed data set and PCA effectively to identify distinct mixing components in the groundwater chemistry
 - Confidence in the paleohydrology mixing model also supports SKB modelling of groundwater chemistry evolution during future events
- The observed late-stage minerals in fractures do not clearly support the predictions of the paleohydrology model
 - Thin and simple Stage 4 mineral coatings
 - Paleohydrology predicts large-scale and repeated changes in groundwater chemistry

Review findings: Groundwater chemistry modelling

- SKB used site characterization data effectively to inform models describing how groundwater chemistry is likely to change under specific future conditions
 - Comprehensive use of site data in modelling for temperate conditions, which was closely tied to the 5 end-member groundwaters
 - However, validity of results is closely tied to validity of groundwater flow models
 - Combined groundwater flow and geochemical equilibrium modelling (PHREEQC)
 - The method provided useful 3D visualizations of site-wide spatial and temporal changes in water chemistry that helped describe the system evolution
 - The method produced thousands of model-generated data points for a statistical analysis of compositional variation at the repository horizon level
 - Conceptual uncertainties for glacial cycle conditions are greater
 - Integration and validation of modelled results will require more detailed review

Recommendations for main review

- Conduct detailed review of SKB's models and reasoned arguments for redox conditions and the potential for deep oxygenated recharge
 - SKB has flagged the persistence of reducing conditions as a significant factor in supporting a key safety function, but effects of glaciations have greatest uncertainties
 - Accordingly, a careful review of the SKB approach is advised
- Assess how SKB has addressed cumulative uncertainties between groundwater flow models and geochemical modelling
- Contrast SKB's site fracture mineralization data with SKB's modelled (PHREEQC) predictions of precipitated mineral phases and their proportions

Requests for supplemental information from SKB

- Provide more information to support SKB's exclusion of cation exchange processes in the PHREEQC modelling
 - Affects the "ionic strength" safety function
- Describe how the Littorina Sea acquired its initial high salinity
 - This bears on whether such a process is expected to recur in future glacial cycles in Sweden
- Assess the current large uncertainties about geochemical processes beneath ice sheets and in permafrost conditions with respect to recent information that is being generated by ongoing field investigations such as the Greenland Analogue Project
 - Data are scarce and uncertain for these conditions, so all new data is of potential relevance to SKB assumptions
- Provide data to confirm deep saline environment at Forsmark or present discussion as to why this is not needed

Recommendations on independent work

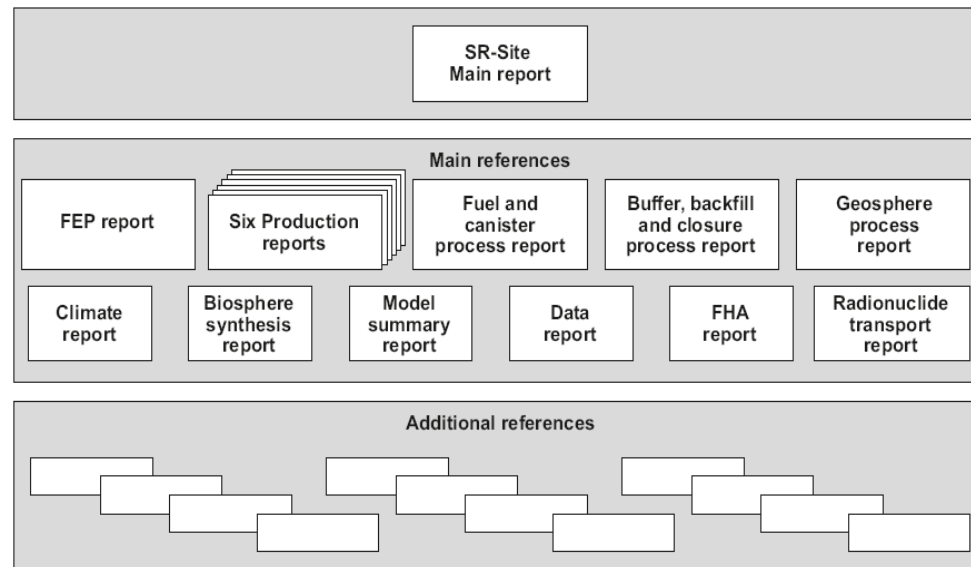
- Conduct a simplified set of confirmatory modelling calculations (mixing and mineral equilibration) to assess the significance of mineral precipitation in altering the modelled evolution of groundwater chemistry
- Perform a detailed modelling analysis to assess the cumulative uncertainties between SKB's groundwater flow models for temperate and glacial cycle periods and the geochemical modelling used to describe the evolution of groundwater chemistry

Additional questions and comments

- SKB's conceptual models describe a dynamic past and future setting for repeated large-scale changes in water chemistry at the Forsmark site (deep meteoric recharge, upwelling of saline waters, submergence by fresh and marine waters, etc.).
 - If so, why is the Stage 4 fracture mineralization so sparse (thin coatings) and texturally simple?
- Describe whether or how SKB has addressed the potential persistence of a microbial “sulfide bloom” (stimulated by sulfate reduction) due to site characterization and construction activities

Additional questions and comments

- SKB states that their hierarchy of the main and additional references to SR-Site includes about 80 additional references (e.g., TR-10-52, p. 12). But how and where are these specific “additional references” identified?
 - How can the reviewers consider these additional references as “endorsed” material that support the safety report if we don’t know which ones they are?



Backup slides

Key documents reviewed (all or in part)

- TR-11-01: Main report
- TR-10-52: Data report
- TR-10-48: Geosphere process report
- TR-08-05: Site description – Forsmark
- TR-10-39: Sulphide content (Tullborg, et al.)
- TR-10-57: Oxygen ingress (Sidborn, et al.)
- TR-10-58: Hydrogeochemical evolution (Salas, et al.)
- R-08-47: Bedrock hydrogeochemistry (Laaksoharju, et al.)
- R-08-84: Explorative analysis of major components and isotopes (Smellie et al.)
- R-08-86: Water-rock interaction modelling (Gimeno, et al.)
- R-08-87: Background complementary hydrogeochemical studies (Kalinowski, ed.)
- R-08-102: Fracture mineralogy (Sandstrom, et al.)

Regulatory framework and safety functions

SSMFS 2008:21 -- “The function of each barrier shall be to, in one or several ways, contribute to the **containment**, prevention, or **retardation** of dispersion of radioactive substances, either directly, or **indirectly** by protecting other barriers in the barrier system.”

- Geosphere (R1) Safety Function: Provide chemically favourable conditions
 - a) **Reducing environment** (*canister corrosion, spent fuel, solubilities, K_d s*) -- **a key repository safety function**
 - b) Salinity (TDS) ... not too high (*buffer and backfill stability, e.g. swelling capability*)
 - c) Ionic strength ... not too low (*buffer and backfill stability, e.g. erosion*)
 - d) Limited concentrations of HS^- , H_2 , CH_4 , organic C (*canister corrosion*), and K^+ and Fe (*buffer and backfill stability*)
 - e) pH less than 11 (*e.g., buffer and backfill stability*)
 - f) Avoid conditions where pH >4 or $[\text{Cl}^-] < 2\text{M}$ (*canister corrosion*)

Output from SKB's geochemical modelling approach

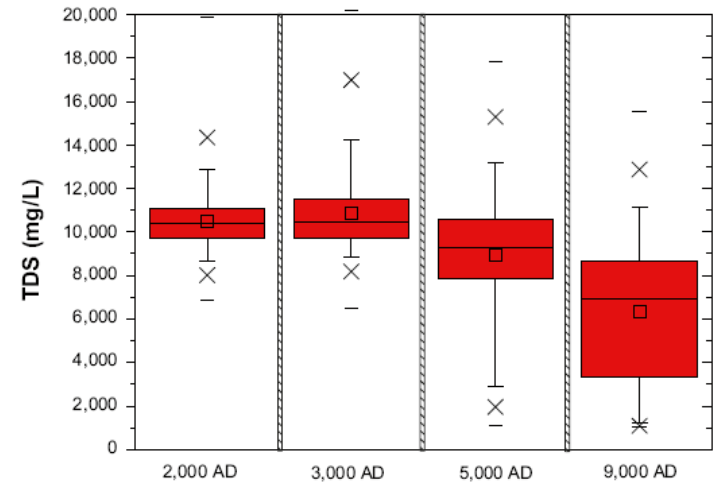
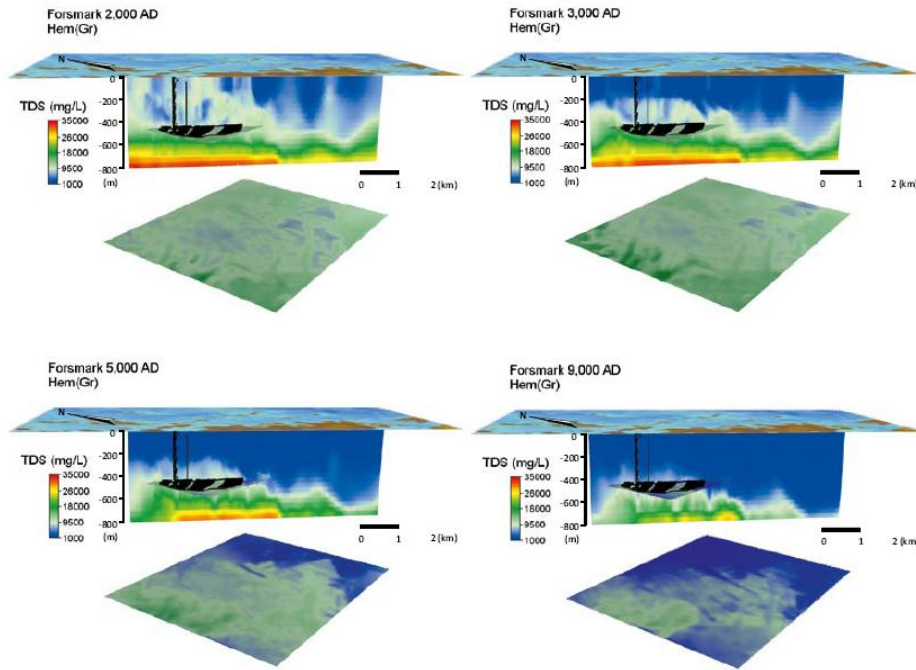


Figure 6-1. Distribution of the computed salinity (TDS in mg/L), for Forsmark in vertical slices at times equal to 2,000 AD, 3,000 AD, 5,000 AD and 9,000 AD.

Examples from SKB's temperate climate evolution case (TR-10-58: Salas, et al.)

Conceptual model for Forsmark after the last glaciation

Pervasive changes in water chemistry over time

- Deglaciation of the site (retreat of ice)
- Submerged site (freshwater lake)
- Submerged site (Littorina Sea, high salinity)
- Uplift and emergence above sea level (present-day conditions)

(Figure 2-17 from Laaksoharju, et al., 2008, SKB report R-08-47)

