Document ID	Version	Status	Reg no	Page
1416882	1.0	Godkänt		1 (3)
Author Luis F. Auqué Patricia Acero Maria J. Gimeno Javier Gómez			Date 2013-11-12	
Reviewed by			Reviewed date	
Approved by Allan Hedin			Approved date 2013-12-19	

Why components that have been measured during the site investigations have been excluded from the SR-Site calculations

The selection criteria adopted to perform the geochemical modelling were to include all those components that significantly contribute or influence the main geochemical characters of the groundwaters (salinity, pH, redox state, etc.) during their natural evolution, and also to include additional components that may have detrimental effects on the safety of the repository.

The analysed components in the Forsmark groundwaters during the site investigation (Laaksoharju et al. 2008) are listed in Table 1 indicating the components included and excluded from the geochemical modelling for SR-Site performed by Salas et al. (2010).

As shown in the table, most of the major and minor components have been considered in the geochemical modelling whilst all trace elements, except aluminium, have been excluded.

Table 1. Analysed components that appear in the table of chemical data from the Forsmark SDM, version 2.2-2.3. Components included and excluded from the geochemical modelling work are indicated.

	Included in calculations	*Excluded from calculations*
Major and minor components	Na, K, Ca, Mg, alkalinity (total inorganic carbon, C_{tot}), SO_4^{2-}, Cl, Br, F, Si, Li, Sr, P, Fe, Mn, S^{2-}	I, DOC, TOC, NO_2^-, NO_3, NH_4^+
Trace elements	Al	As, B, Ba, Cd, Cr, Cu, Co, Hg, Mo, Ni, Nb[1], Pb, V, Zn. Zr, U, Th, Sc, Rb, In, Sb, Cs, Y, REE (La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu) Hf, Tl

Trace elements

Contents of all trace elements are in the microgram/L or nanogram/L range (e.g. most of the analytical values for Co, Cr, Cu, Pb, Sb, V and REE) and some of them occur most frequently at concentrations below the detection limit (Th, In, Hf, Tl, Cd, Sc, Hg and heavy REE) in uncontaminated groundwater systems.

[1] Nb is listed in the table from SDM 2.2-2.3 but there are no analytical data for this element.

Svensk Kärnbränslehantering AB
Swedish Nuclear Fuel and Waste Management Co
PO Box 250, SE-101 24 Stockholm
Visiting address Blekholmstorget 30
Phone +46-8-459 84 00 Fax +46-8-579 386 10
www.skb.se
556175-2014 Seat Stockholm

Aluminium has been the only element of this group of trace metals included in the geochemical calculations. Although its concentration is very low under neutral-basic conditions, aluminium is involved in heterogeneous reactions with aluminosilicate minerals and, thus, it may participate in the control of some groundwater characteristics (e.g. pH). The rest of the trace elements have not been considered in the calculations due to the following reasons:

- In contrast with aluminium, they are not involved in the control of any important compositional system for the evolution of the groundwaters.
- Their very low concentrations would preclude significant influences on the "major" compositional systems (e.g. the carbonate system) through speciation reactions or activity coefficient calculations (their influence in the ionic strength, a critical parameter for the activity coefficient calculations, is minimal, if any).
- Also, because of their low concentrations, their contribution to the groundwater salinity is negligible.

All these circumstances would also explain why none of the excluded trace elements has been considered in the selected reference groundwaters used in previous risk assessments, *e.g.* SKI-94 (SKI 1996, Table 10.4.1), SR-97 (SKB 1999, Tables 8.7, 8.8 and 8.9), or Sr-Can (Auqué et al. 2006, Table 2-1), or in predictive calculations carried out by other authors and related to the natural evolution of groundwaters (*e.g.* Molinero et al. 2008, Tables 2–4, Bath 2011, Tables 1 and 2).

Major and minor components

As stated above (see also Table 1), most of the major and minor components have been considered in the geochemical modelling, since they have been included in the end-members used for the mixing and reaction calculations (see Table 4-2 and Appendix 1 in Salas et al. 2010). The excluded components are Iodine, DOC (dissolved organic carbon), TOC (total organic carbon), NO_2^-, NO_3^- and NH_4^+ due to the following reasons:

- Iodine (I) is presently found in very low amounts in the Forsmark groundwaters (in the microgram/L range, with a mean value around 100 µg/L) and neither participates in the control of important hydrochemical characters nor shows detrimental effects for the repository performance.
- DOC, TOC, NO_2^-, NO_3^- and NH_4^+ cannot be modelled in the same way and with the same tools as the rest of the geochemical parameters because their evolution is closely related to the microbial activity. However, these components may have detrimental effects on the repository performance (e.g. by enhancing sulphate reduction or some specific types of canister corrosion). Thus, they have been qualitatively evaluated in the work carried out for SR-Site (see Section 8 Evaluation of other geochemical parameters in Salas et al. 2010) and in the corresponding modelling for Laxemar (see Section 5, Evolution over time of other geochemical parameters in Gimeno et al. 2010). Although there are large uncertainties concerning the concentrations of these components along a glacial cycle, the evaluation for Forsmark was that the expected concentrations would not affect the long term safety of the proposed repository (cf. Table 8-1 in Salas et al. 2010).

Overall, all the components included in this category (except iodine) have been considered in the hydrochemical evaluation presented by Salas et al. (2010) and most of them have also been included in the modelling calculations, at least, to take into account their effects on salinity.

References

Auqué L F, Gimeno M J, Gómez J, Puigdomenech I, Smellie J, Tullborg E-L, 2006. Groundwater chemistry around a repository for spent nuclear fuel over a glacial cycle. Evaluation for SR-Can. SKB TR-06-31, Svensk Kärnbränslehantering AB.

Bath A, 2011. Infiltration of dilute groundwaters and resulting groundwater compositions at repository depth. Report 2011:22, Strålsäkerhetsmyndigheten (Swedish Radiation Safety Authority).

Gimeno M J, Auqué L F, Gómez J B, Salas J, Molinero J, 2010. Hydrogeochemical evolution of the Laxemar site. SKB R-10-60, Svensk Kärnbränslehantering AB.

Laaksoharju M, Smellie J, Tullborg E-L, Gimeno M, Hallbek L, Molinero J, Waber N, 2008. Bedrock hydrogeochemistry Forsmark. Site descriptive modeling, SDM-Site Forsmark. SKB R-08-47, Svensk Kärnbränslehantering AB.

Molinero J, Raposo J R, Galíndez J M, Arcos D, Guimerá J, 2008. Coupled hydrogeological and reactive transport modelling of the Simpevarp area (Sweden). Applied Geochemistry 23, 1957–1981.

Salas J, Gimeno M J, Auqué L, Molinero J, Gómez J, Juárez I, 2010. SR-Site – hydrogeochemical evolution of the Forsmark site. SKB TR-10-58, Svensk Kärnbränslehantering AB.

SKB, 1999. Deep repository for spent nuclear fuel. SR 97 – Post-closure safety. Main report. SKB TR-99-06, Svensk Kärnbränslehantering AB.

SKI, 1996. SKI Site-94. Deep repository performance assessment project. SKI Report 96:36, Statens kärnkraftinspektion (Swedish Nuclear Power Inspectorate).