Verification/validation of the codes PHREEQC, PHAST and TOUGHREACT

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This document complements the information in SR-Site (Model Summary Report, TR-10-51) concerning QA related issues regarding the codes PHREEQC, PHAST and TOUGHREACT, raised by SSM in a request for additional information to that given in the safety assessment SR-Site (reference SSM2011-2426-80).

1 PHREEQC

PHREEQC is a free geochemical modelling tool (non-commercial, open source), which is developed and maintained by the USGS (United States Geological Survey). It is the culmination of a development policy initiated by the USGS in the sixties to develop geochemical tools. PHREEQC has become a modelling environment in which various modelling techniques have been introduced and improved that previously used to be separate USGS programs, including some of the most used in the eighties and nineties, such as WATEQ4F, PHREEQE and NETPATH.

Because it is so wide-spread, and due to the USGS's policy of constant maintenance and updating, there has been continuous feedback loop between users and developers: problems or errors have been detected quickly in new versions, resulting in quick and efficient corrections. This means that PHREEQC is possibly one of the more refined and widely used programs that currently exist. E.g. Google Scholar has more than 5000 references that use or cite PHREEQC. A confirmation that the program produces correct results is found in references that present comparisons of results between PHREEQC and other codes (De Windt et al. 2003, Gundogan et al. 2011, Nowack et al. 2006, Schüßler et al. 2001), as well as in some verification calculations reported in the user's manual.

PHREEQC can be freely downloaded from the USGS website (June 14, 2013):
http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc/
On this website, under the heading "Status of PHREEQC Programs", a complete list of enhancements, changes and bug fixes that have been performed in the different versions of this code is available. The source is, therefore, public and completely and transparently traceable.

Therefore SKB considers PHREEQC to be sufficiently verified for the purposes of SR-Site, i.e. equilibria in groundwater and with a few specific minerals. PHREEQC is adequate for such type of equilibrium and mixing calculations as evidenced in the manual and by the extensive number of peer-reviewed publications that use this code; a representative example is provided by Rebeix et al. (2011).

References not included in SKB's licence application

De Windt L, Burnol A, Montarnal P, van der Lee J, 2003. Intercomparison of reactive transport models applied to UO_2 oxidative dissolution and uranium migration. Journal of Contaminant Hydrology 61, 303–312.

Gundogan O, Mackay E, Todd A, 2011. Comparison of numerical codes for geochemical modelling of CO_2 storage in target sandstone reservoirs. Chemical Engineering Research and Design 89, 1805–1816.

Nowack B, Mayer K U, Oswald S E, van Beinum W, Appelo C A J, Jacques D, Seuntjens P, Gérard F, Jaillard B, Schnepf A, Roose T, 2006. Verification and intercomparison of reactive transport codes to describe root-uptake. Plant and Soil 285, 305–321.

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Rebeix R, Le Gal La Salle C, Michelot J-L, Verdoux P, Noret A, Monvoisin G, Gianesinni S, Lancelot J, Simler R, 2011. Tracing the origin of water and solute transfers in deep groundwater from Oxfordian, Dogger and Trias formations in the east of the Paris Basin – France. Physics and Chemistry of the Earth, Parts A/B/C 36, 1496–1510.

Schüßler W, Artinger R, Kim J I, Bryan N D, Griffin D, 2001. Numerical modeling of humic colloid borne americium (III) migration in column experiments using the transport/speciation code K1D and the KICAM model. Journal of Contaminant Hydrology 47, 311–322.

2 PHAST

PHAST is a free geochemical modelling tool (non-commercial, open source), which is developed and maintained by the USGS (United States Geological Survey). It is relatively wide-spread, Google Scholar has more than 200 references that use, or cite, PHAST. Release notes available from the USGS website report changes between versions.

Verification of the code is included in the seven examples described in the manual (Parkhurst et al. 2010).

This type of reactive transport modelling tools are appropriate for fractured rocks (MacQuarrie and Mayer 2005) as well as for saturated bentonite-groundwater interactions (Arcos et al. 2003). Therefore PHAST is adequate for its use in SR-Site, that is, modelling of oxygen ingress in granite fractures and modelling of water-saturated bentonite interaction with groundwater.

References included in SKB's licence application

Arcos D, Bruno J, Karnland O, 2003. Geochemical model of the granite–bentonite–groundwater interaction at Äspö HRL (LOT experiment). Applied Clay Science 23, 219-228.

MacQuarrie K T B, Mayer K U, 2005. Reactive transport modeling in fractured rock: a state-of-the-science review. Earth-Science Reviews, 72, 189–227.

References not included in SKB's licence application

Parkhurst D L, Kipp K L, Charlton S R, 2010. PHAST Version 2 – A program for simulating groundwater flow, solute transport, and multicomponent geochemical reactions. Techniques and Methods 6-A8, U.S. Geological Survey Denver, Colorado.

3 TOUGHREACT

This is a widely used commercial code developed at the LBNL. TOUGHREACT was used in SR-Site for the modelling of reactive transport in the buffer. TOUGHREACT is appropriate for this type of models as described in its documentation and several publications, for example Itälä et al. (2011) and Arthur and Zhou (2005).

Gundogan et al. (2011), Pruess et al. (2004) and Xu et al. (1999) describe either the verification, or inter-code comparison of TOUGHREACT.

References included in SKB's licence application

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Arthur R, Zhou W, 2006. Reactive-transport model of buffer cementation. SKI Report 2005:59, Statens kärnkraftinspektion (Swedish Nuclear Power Inspectorate).

References not included in SKB's licence application

Gundogan O, Mackay E, Todd A, 2011. Comparison of numerical codes for geochemical modelling of CO_2 storage in target sandstone reservoirs. Chemical Engineering Research and Design 89, 1805–1816.

Itälä A, Olin M, Lehikoinen J, 2011. Lot A2 test, THC modelling of the bentonite buffer. Physics and Chemistry of the Earth, Parts A/B/C 36, 1830–1837.

Pruess K, García J, Kovscek T, Oldenburg C, Rutqvist J, Steefel C, Xu T, 2004. Code intercomparison builds confidence in numerical simulation models for geologic disposal of CO_2. Energy 29, 1431–1444.

Xu T, Pruess K, Brimhall G, 1999. An improved equilibrium-kinetics speciation algorithm for redox reactions in variably saturated subsurface flow systems. Computers & Geosciences 25, 655–666.

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