



Public

Memo

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Documentation of the code for erosion and corrosion calculations in SR-Site

1 Introduction

This document describes the computer code used for calculations of buffer erosion and copper canister corrosion (by corroding agents in groundwater) in the safety assessment SR-Site. The computer code is a Microsoft Excel workbook, consisting of a number of work sheets.

In the following, references on the formats TR-xx-xx and R-xx-xx refer to SKB reports of the TR and R series, respectively. All these are available at www.skb.se. Most of the mathematical models implemented in the code are described in SKB TR-10-66.

2 Version

This document describes version 1.0 of the code, with file name ErosionCorrosionModel_1_0.xlsx, stored under ID 1265612 in SKB's document management system SKBdoc. This version is identical to version 0.8 except that additional comments have been inserted in the code, that some minor restructuring has been done to enhance clarity and that some parts not used in SR-Site were deleted. Version 0.8 was used for most of the final calculations in SR-Site. Earlier versions were used in preliminary calculations and in the development work. Version 0.7 was used for some of the sensitivity calculations presented in TR-10-66. Version 0.9 was used for investigation of a particular detail for the case of diffusive transport in the buffer, as also documented in TR-10-66. The development of the code is described in the sheet "History".

3 Implemented mathematical models

The code is used to calculate

- buffer erosion;
- canister corrosion by sulphide in groundwater, for advective conditions in the eroded buffer; and
- canister corrosion by sulphide in groundwater, for diffusive conditions in an intact buffer.

The code can also be used to calculate corrosion due to oxygen (and other corroding agents) by modifying the input parameters relating to sulphide. A version of the model dedicated to SR-Site calculations of corrosion caused by oxygen in the groundwater for advective conditions in deposition holes is described in Appendix 3.

The code could also be used to quantify corrosion processes limited by outward transport of soluble corrosion products.

All these calculations use hydrogeological data for the entire ensemble of deposition holes in the repository, with optional application of a number of deposition position rejection criteria.

3.1 The erosion model

Using the nomenclature in TR-10-66, section 4.3.1, the erosion rate, $R_{Erosion}$, as derived in TR-09-35 is proportional to the water velocity, v , to the power 0.41 and directly proportional to the size of the fracture aperture, δ , according to

$$R_{Erosion} = A_{ero} \cdot \delta \cdot v^{0.41} \quad (1)$$

where the exponent 0.41 and the constant $A_{ero} = 27.2$ (yielding the loss rate in kg/yr when the water velocity is given in m/yr and the aperture in m) are fitted data given in TR-10-64, Equation 5-1.

The time to reach advective conditions in the buffer, t_{adv} , is given by

$$t_{adv} = \frac{m_{buffadv}}{R_{Erosion} \cdot f_{tdilute}} \quad (2)$$

where $m_{buffadv}$ is the amount of buffer mass loss required to reach advective conditions, and $f_{tdilute}$ is the fraction of time with groundwater sufficiently dilute for erosion.

The value of the aperture δ is obtained from the data file from the hydrogeological modelling, and the velocity v of the flowing water in the fracture intersecting the deposition hole is obtained from U_0 in the same file as

$$v = U_0 \frac{h_{can}}{\delta} \quad (3)$$

This expression is obtained by inserting Q_f from Equation 3-8 in R-09-20 into Equation D-7 in the same report. It is then also noted that *i*) the fluxes from the possibly several fractures intersecting the deposition hole are pessimistically summed to a total flux and *ii*) the height of the canister, h_{can} , corresponds to the entity w in R-09-20 (see text in connection to Equation 3-8 in R-09-20). The parameter value $w = h_{can} = 5$ m is used by Serco in deriving U_0 from the volumetric flow rate in the fracture, and the same value should thus be used in Equation 3 to obtain v by back calculating the volumetric flow rate.

3.2 The corrosion model for advective conditions in the buffer

The rate of corrosion once advective conditions are reached in the buffer, v_{corr} , is given in TR-10-66, section 4.3.2, as

$$v_{corr} = Q_{eq} \cdot [HS^-] \frac{f_{HS} M_{Cu}}{\rho_{Cu}} \frac{1}{A_{corr}} \quad (4)$$

where Q_{eq} is the equivalent flowrate, $[HS^-]$ is the concentration of sulphide in the groundwater in the fracture, $f_{HS} = 2$ is a stoichiometric factor taking into account the reaction of sulphide with copper, M_{Cu} is the molar mass of copper, ρ_{Cu} is the density of copper and A_{corr} the area exposed to corrosion.

The time, t_{Corr} , required to corrode through a canister wall of thickness d_{can} is thus

$$t_{corr} = \frac{d_{can}}{v_{corr}} = \frac{d_{can} \cdot A_{corr}}{Q_{eq} \cdot [HS^-] f_{HS} M_{Cu}} \frac{\rho_{Cu}}{M_{Cu}} \quad (5)$$

A_{corr} is given in TR-10-66, section 4.3.3 as

$$A_{corr} = \pi r_{can} h_{corr} \quad (6)$$

where r_{can} is the canister radius and h_{corr} is the height of the canister exposed to corrosion.

Q_{eq} for an eroded buffer is given in TR-06-33, chapter 6: For small flow rates, Q_{eq} equals the flow rate through the eroded buffer, q_{eb} . For sufficiently large flow rates, Q_{eq} varies as the square root of q_{eb} according to

$$Q_{eq} = \frac{1.13 \sqrt{q_{eb} D_w V_{zone}}}{d_{buffer}} \quad (7)$$

where D_w is the diffusion coefficient of solute in water, V_{zone} is the volume of the eroded buffer and d_{buffer} is the thickness of the buffer. In the Appendix to TR-10-42, it is also demonstrated that the smaller of the two expressions for Q_{eq} gives the better approximation irrespective of the magnitude of the flow rate, meaning that the linear expression should be used for $q_{eb} < q_{lim}$ where /TR-10-42, Appendix/

$$q_{lim} = \left(\frac{1.13}{d_{buffer}} \right)^2 D_w V_{zone} \quad (8)$$

V_{zone} is given in TR-10-66, section 4.3.3 as

$$V_{zone} = h_{zone} \pi (r_h^2 - r_{can}^2) / 2 \quad (9)$$

where h_{zone} is the height of the eroded zone set equal to d_{buffer} and r_h is the radius of the deposition hole. However, a preliminary, now obsolete and more pessimistic version of Equation (9) was erroneously implemented in all versions of the code up to and including v 1.0:

$$V_{zone} = h_{zone} \pi (r_h^2 - r_{can}^2) \quad (9a)$$

This expression was hence used in the calculations in SR-Site. In Appendix 1 to this Memo, it is demonstrated that Equation (9a) gives *i*) a slightly lower probability of canister failure due to corrosion and *ii*) a slightly lower calculated dose consequence than Equation (9).

The hydrogeological modelling in SR-Site gives the Darcy flux U_0 at a deposition position as output and this is related to q_{eb} as

$$q_{eb} = f_{conc} U_0 2r_h h_{can} \quad (10)$$

where f_{conc} is a flow concentration factor accounting for a flow increase caused by the cavity in the buffer intersecting the water conducting fracture and h_{can} corresponds to the entity w in /R-09-20, Equation (3-8)/ as explained in conjunction with Equation (3) above.

3.3 The corrosion model for diffusive conditions in the buffer

This model is obtained from the expressions in TR-10-66 as explained in section 4.6.5 below.

4 Workbook structure

The Excel workbook consists of a number of spreadsheets as described in the following subsections.

4.1 Info

The sheet “Info” contains

- settings for the various calculation cases, allowing specification of input data files from hydrogeological calculations, filtering options etc (blue cells)
- key outputs (yellow cells)
- model parameters; these are data in the implemented mathematical models for erosion and corrosion for the KBS-3 design and that are normally the same in all calculation cases (green cells)

The contents of this sheet are not further documented here; the reader is referred to the detailed comments in the work sheet and references therein.

4.2 @Risk

The sheet “@Risk” contains information for automatic running of multiple cases consecutively, using the Excel plug-in programme @Risk, and yielding identical results as with manual running. The option is toggled on or off in sheet “Info”. The @Risk functions are disabled in v 1.0, but were used to increase calculation speed at some stages of the SR-Site work.

4.3 HSData

The sheet “HSData” contains four tables of sulphide concentration data: “HSGeneric”, “HSForsmark”, “HSLaxemar” and “HSTest”. The tables are defined as Excel Names, meaning that they are accessible globally in the workbook. The selection of a specific table for a calculation case is made in the sheet “Info”.

4.4 fs_Q1_2000_pline_merged

The sheet “fs_Q1_2000_pline_merged” contains hydrogeological output from the base case calculation with the semi-correlated hydrogeological DFN model, see further R-09-20, section 4.3. This case is used also in many base case calculations of erosion and corrosion. Alternative hydrogeological data files must be structured like the one in sheet “fs_Q1_2000_pline_merged”.

To use hydrogeological data from another file in the calculations, that file must be open in Excel and the file and sheet name given in sheet "Info"

4.5 InflowReject

The sheet "InflowReject" contains data from calculations of inflow to deposition holes under simulated open repository conditions for the semi-correlated hydrogeological base case of the Forsmark site. Several calculations were made with differing assumptions regarding grouting of deposition holes and regarding flow related rejection criteria, see further R-09-19 for a description of the inflow calculations. These data are used if the option "Filtering of high inflow holes?" in sheet "Info" is selected. In SR-Site, this option is only used to elucidate the potential impact of flow related rejection criteria that may be developed in later stages of the repository development.

4.6 Calc

The sheet "Calc" contains all calculations done in the Workbook. Each row represents one deposition position according to the repository layout represented in the selected data file from the hydrogeological modelling. The sheet is set up to handle hydrogeological data files representing up to 10,000 deposition positions.

The calculations made in each of the columns are described in the following.

4.6.1 Columns C through N

The blue columns C through L are copied from the selected hydrogeological data file without any processing. These columns are used as input to the erosion and corrosion calculations. The column N contains data from hydrogeological modelling of an open repository. The column contents are briefly described in the following.

- C This column contains the number index of the deposition position for each row. The sheet is set up to handle hydrogeological data files representing up to 10,000 deposition positions. If the data file contains $NCAN < 10,000$ positions, the number index in column C is set to zero in the excess positions.
- D This column contains information on the so called OKFLAG in the hydrogeological modelling. If $OKFLAG \neq 0$, this denotes a deviation from expected behaviour of the hydrogeological model, as further described in R-09-20, Appendix B.
- E This column contains the calculated values of the Darcy flux in a fracture intersecting the deposition position in the hydrogeological modelling. This entity is denoted U0 in the hydrogeological modelling, see further R-09-20, Appendix B.
- F This column contains the calculated values of the equivalent flow rate in a fracture intersecting the deposition position in the hydrogeological modelling. This entity is denoted QEQ in the hydrogeological modelling, see further R-09-20, Appendix B.
- G This column contains the calculated values of the advective travel time from the deposition position to the surface for a particle starting in a fracture intersecting the deposition position in the hydrogeological modelling. This entity is denoted TW in the hydrogeological modelling, see further R-09-20, Appendix B.

- H This column contains the calculated values of the flow related transport resistance from the deposition position to the surface for a path starting in a fracture intersecting the deposition position in the hydrogeological modelling. This entity is denoted F in the hydrogeological modelling, see further R-09-20, Appendix B.
- I This column contains the values of the transport aperture in a fracture intersecting the deposition position in the hydrogeological modelling. This entity is denoted TRAPP in the hydrogeological modelling, see further R-09-20, Appendix B.
- J This column indicates whether a deposition position fulfils the so called full perimeter intersection criterion, FPC. $FPC \neq 0$ means that the criterion is fulfilled. See further R-09-20, Appendix B.
- K This column indicates whether a deposition position is fully intersected by a fracture. The number in this column indicates the number of adjacent positions that are also fulfilled by this fracture. This information is used to determine if a deposition position fulfils the so called extended full perimeter intersection criterion, EFPC. See further R-09-20, Appendix B.
- L This column contains the values of the length of the largest fracture intersecting the deposition position in the hydrogeological modelling. This entity is denoted FLEN in the hydrogeological modelling, see further R-09-20, Appendix B.
- M This column is blank.
- N This column is copied from the sheet "InflowReject" and contains data to be used if deposition positions are rejected based on inflow criteria. With the default settings used in SR-Site, this rejection criterion is not used.

4.6.2 Columns P through AA

The yellow columns P through AA contain calculated entities based on copied data, with each row corresponding to a particular deposition position, according to the following.

- P In this column, the alternative pessimistic fracture aperture $\delta = 0.275 \cdot (\text{TRAPP}/0.5)^{2 \cdot 0.297}$ is calculated. This aperture is used in the quantification of erosion if the pessimistic aperture option is selected in sheet "Info". Otherwise TRAPP is taken from hydrogeological input data, see further TR-11-01, section 12.2.2, p 579.

- Q In this column, the transmissivity T of a fracture intersecting a deposition hole is back calculated from the transport aperture TRAPP as /TR-09-20, Equation 3-2/

$$T = \left(\frac{\text{TRAPP}}{0.5} \right)^2$$

where TRAPP is given in m and T in m^2/s . The calculated transmissivities are not further used in SR-Site.

- R In this column, the gradient i [m/m] is calculated from the Darcy flux U_0 and the transmissivity T converted to m^2/yr according to

$$i = \frac{U_0 h_{can}}{T}$$

The calculated gradients are not further used in SR-Site.

- S In this column, the water velocity v is calculated according to Equation (3) above.

- T In this column, the time to reach advective conditions in the buffer, t_{adv} , is calculated according to Equation (2) above. If either the deposition hole is rejected according to the selected criteria for rejection (see description of column Z below) or $v = 0$, t_{adv} is set to $1E+99$.
- U In this column, the flow rate through an eroded deposition hole, q_{eb} , is calculated according to Equation (10) above. This entity is denoted q in the code.
- V In this column, the minimum sulphide concentration required to obtain corrosion failure within a set time, $T_{FailFilteringLim}$, with a default value of 1,000,000 years (set in sheet "Info"), is calculated. The time taken to reach advective conditions is accounted for so that t_{corr} is set to $T_{FailFilteringLim} - t_{adv}$. The minimum sulphide concentration is then obtained by solving Equation (5) above for $[HS^-]$. If either $q = 0$ or t_{corr} is negative the minimum sulphide concentration is set to $1E+99$.
- W In this column, the minimum time of failure due to corrosion is calculated by applying the highest sulphide concentration in the selected distribution to Equation (5) above. The value of t_{adv} is included in the failure time. If either t_{adv} (column T) or the minimum sulphide concentration (column V) was set to $1E+99$ or if t_{corr} is negative the minimum failure time is set to $1E+99$.
- X In this column, the number of data points in the distribution of sulphide concentrations that can cause corrosion failure within $T_{FailFilteringLim}$ is determined by counting the number of data points exceeding the value calculated in column V.
- Y In this column, it is determined if the deposition position in question is a so called EFPC edge position. An edge position is partially intersected by a large fracture that causes EFPC rejection of adjacent deposition positions, but not in the current position according to the definition of the EFPC. This information is not further used in the calculations.
- Z In this column, it is determined if the deposition position in question is rejected according to any of the rejection criteria selected in sheet "Info". These criteria relate to fracture geometry or flow conditions that would in principle be observable during the construction of the repository.
- AA In this column, it is determined if the deposition position in question is omitted from further calculations, for any of the following reasons:
- the position is rejected according to column Z
 - the row number is higher than the number of deposition positions in the layout (meaning that column C is zero)
 - the calculated minimum failure time in column W exceeds the set limit $T_{FailFilteringLim}$
 - the OKFLAG in column D $\neq 0$ and the OKFLAG filtering option is selected.

4.6.3 Columns AC through AH

In the orange columns AC through AH data are filtered so that only data to be propagated to radionuclide transport calculations remain. This means that the deposition positions that are omitted according to column AA are filtered out, yielding a "compressed" table starting in column AF.

- AC The value in this column is equal to that in column X, except that it is set to zero if the deposition position is omitted according to column AA.
- AD In this column, each row is assigned an order number. If the first row is to be included after filtering (i.e. if it has a non-zero value in column AC) it is assigned the order number one, otherwise zero. If a subsequent row is to be included after filtering, it obtains a number that is one unit higher than that of the previous row, otherwise it obtains the same number as the previous row. (The result is used to construct a “compressed” table, starting in column AF.)
- AE The value in this column is equal to that in column C (the deposition position ID number), except that it is set to zero if the deposition position is omitted according to column AA.
- AF This column contains the deposition position ID numbers of only the positions remaining after filtering, in ascending order. Normally only a few of the typically more than 6,000 depositions positions remain. All rows set to zero in column AE are thus omitted here and a “compressed” version of column AE, with only the non-zero values remaining, is obtained.
- AG This column contains the information from column X for the positions remaining after filtering, i.e. those listed in column AF.
- AH This column is a cumulative summation of the data in column AG. The first cell in column AH has the value 1.

4.6.4 Columns AJ through AR

In the green columns AJ through AR are used to construct a list of canister failure times for the positions where failure was calculated to occur. Each data point in the distribution of sulphide concentrations that lead to canister failure generates a failure time for a given canister position.

- AJ This column is a copy of column AF, as it is convenient to have this info next to the subsequent column.
- AK This column contains the deposition position ID numbers of the positions remaining after filtering, in ascending order. Each such deposition number is repeated as many times as there are data points in the sulphide distribution generating a failure time.
- AL This column contains the index numbers in the sulphide table generating failure times according to column AK.
- AM This column contains the calculated values of t_{adv} for the canister positions in column AK.
- AN This column contains the sulphide concentrations corresponding to the sulphide table indices in column AL.
- AO This column contains the calculated values of the flow rate through the eroded deposition position, q , for the canister positions in column AK. The q -values are those calculated in column U.
- AP This column contains the calculated corrosion times with the sulphide concentration in column AN and the q -values in column AO.
- AQ This column contains the calculated failure times, i.e. the sum of erosion and corrosion times in columns AM and AP, respectively.

AR This column indicates if a failure time in column AQ occurred for a canister in an EFPC edge position according to column Y. The column is only used for inspection of the calculated results, for cases where edge positions occur.

4.6.5 Columns AU through BE

Columns AU through BE handle corrosion for diffusive conditions. The key calculations are done in columns AU through AY according to the following:

AU This column contains a calculation of the corrosion rate for the case with diffusion through an intact buffer and where the corroding agent (sulphide) is provided from the flowing groundwater in a fracture intersecting the intact deposition hole. The corrosion rate is obtained by solving Equation 4-14 in TR-10-66 for Q_{eq} and inserting the resulting expression in Equation 4-19 in TR-10-66.

AV This column contains a calculation of the flow related equivalent flow rate when thermally induced spalling has affected the wall of the deposition hole, i.e. of $Q_{eqhydro} + Q_{eqspalling}$ where $Q_{eqhydro}$ is obtained directly from the hydrogeological modelling and $Q_{eqspalling}$ is taken from Equations 4-9, 4-11 and 4-12 in TR-10-66.

AW This column contains a calculation of the corrosion rate for the case with diffusion through an intact buffer and where the corroding agent (sulphide) is provided from the flowing groundwater in a fracture intersecting the deposition hole. The walls of the deposition hole are here assumed to be affected by thermally induced spalling. The corrosion rate is that given in Equation 4-19a in TR-10-66. However, in versions of the code up to v 0.9, and hence in the calculations reported in SR-Site, a now obsolete, slightly more pessimistic expression was used. Calculation cases comparing the two expressions are documented in Appendix 2 to this Memo.

AX This column is identical to column AU, except that the corrosion rate for deposition positions rejected according to column Z is set to zero.

AY This column is identical to column AW, except that the corrosion rate for deposition positions rejected according to column Z is set to zero.

Columns BA through BE are used to construct cumulative distributions of the results of the calculations in columns AU through AY.

4.6.6 Remaining columns in sheet Calc

The remaining columns in sheet Calc are used

- to construct cumulative distributions of the QEQ data in column F, and of the same entity with data filtered according to column Z;
- to calculate the erosion rate in each deposition hole according to Equation 1 and construct cumulative distributions of this result, and of the same entity with data filtered according to column Z;
- to calculate the corrosion rate for a fixed sulphide concentration with advective conditions in each deposition hole and construct cumulative distributions of this result, and of the same entity with data filtered according to column Z; and
- to construct cumulative distributions of the gradient i in column R, and of the same entity with data filtered according to column Z.

4.7 QeqPlt

The sheet “QeqPlt” contains a plot of the distribution, taken over the ensemble of deposition holes in the repository, of the equivalent flow rate, as given in the data from the hydrogeological modelling. It is thus a plot of input data to the erosion and corrosion calculations.

4.8 CorrDiffPlt

The sheet “CorrDiffPlt” contains a plot of the distribution, taken over the ensemble of deposition holes in the repository, of the calculated corrosion rates for diffusive conditions in the buffer, and for a constant sulphide concentration.

4.9 EroPlt

The sheet “EroPlt” contains a plot of the distribution, taken over the ensemble of deposition holes in the repository, of the calculated rates of buffer erosion.

4.10 CorrAdvPlt

The sheet “CorrAdvPlt” contains a plot of the distribution, taken over the ensemble of deposition holes in the repository, of the calculated corrosion rates for advective conditions in the buffer, and for a constant sulphide concentration.

4.11 iPlt

The sheet “iPlt” contains a plot of the distribution, taken over the ensemble of deposition holes in the repository, of the calculated hydraulic gradients.

4.12 InputTrptCalcs

The sheet “InputTrptCalcs” contains input data for radionuclide transport calculations resulting from the calculations of erosion and corrosion for advective conditions. It also contains the model parameters used in the calculations, through links to sheet “Info”. The radionuclide transport data are used in consequence calculations for the “Canister failure due to corrosion scenario” in SR-Site, see section 13.5 of TR-11-01 and TR-10-50 for further details.

4.13 History

The sheet “History” describes the development history of the Workbook, up to the present version.

5 Code testing

5.1 Introduction

The code has been tested against the analytical expressions for buffer erosion and canister corrosion throughout the development. For formal testing, a test file with hydrogeological input data has been constructed. It yields an output table to radionuclide transport calculations that is easy readily checked for errors.

To test the code, the hydro data file and worksheet name (cell Calc!C2) should be set to [TestCaseHydro.xlsx]Test and the file TestCaseHydro.xlsx should be opened. The HSTabName (cell Calc!C3) should be set to HSTest. Otherwise all settings and parameters should be unchanged, i.e. they should keep their default values.

The input data file TestCaseHydro.xlsx is designed to provide a verification of the code ErosionCorrosionModel_1_0.xlsx and in particular the output to radionuclide transport calculations for the corrosion scenario in SR-Site.

The input files with data from the hydrogeological modelling contain information, for each deposition hole, on U_0 , δ , etc required for the erosion and corrosion calculations. The input test file is structured as the files emerging from the hydrogeological modelling, and contains data aimed at code testing.

5.2 Data row 1: Testing the corrosion calculation when $q_{eb} < q_{lim}$

The first data row in TestCaseHydro.xlsx is designed to test the corrosion model for a case where $q_{eb} < q_{lim}$ (see section 3.2). In this row, the fracture aperture, δ , is set to an extremely high value ($1E+99$) to render a negligible value of t_{adv} according to Equation (2).

The Darcy flux U_0 is set to a value that yields a corrosion time of 850,000 years for the highest sulphide concentration ($1 \cdot 10^{-4}$ M) in the distribution given in the table HSTest in sheet HSData and with all other parameters set to their default values in the model, i.e.

$$\begin{aligned}d_{can} &= 0.047 \text{ m} \\r_{can} &= 0.525 \text{ m} \\h_{corr} &= d_{buffer} = 0.35 \text{ m} \\f_{HS} &= 2 \\M_{Cu} &= 63.55 \text{ kg/kmoles} \\\rho_{Cu} &= 8920 \text{ kg/m}^3\end{aligned}$$

Inserting these values into Equation (6) and Equation (5) solved for Q_{eq} yields a value of Q_{eq} that can be used to determine U_0 using Equation (10) with

$$\begin{aligned}f_{conc} &= 2 \\r_h &= 0.875 \text{ m} \\h_{can} &= w = 5 \text{ m}\end{aligned}$$

This yields a U_0 -value of $1.28 \cdot 10^{-3}$ m/yr. Note that this corresponds to a q -value lower than q_{lim} , which with

$$\begin{aligned}D_w &= 0.0315 \text{ m}^2/\text{yr} \\h_{zone} &= d_{buffer} = 0.35 \text{ m}\end{aligned}$$

yields a q_{lim} of $0.1769 \text{ m}^3/\text{yr}$ according to Equation (8), corresponding to $U_0 = 1.01 \cdot 10^{-2}$ m/yr. This means that Q_{eq} is taken to equal q_{eb} .

The subsequent values of [HS⁻] in HSTest are set to yield corrosion times increasing in steps of 10,000 years, i.e. the resulting corrosion times are 860,000 years, 870,000 years etc., up to 940,000 years for the lowest sulphide concentration. This row of input data should thus generate ten failure times, being the same as the corrosion times since t_{adv} is negligible, and hence ten lines of output to be used as input to radionuclide transport calculations.

5.3 Data row 2: Testing the corrosion calculation when $q_{eb} > q_{lim}$

The second data row has a similar testing function as the first, except that the Darcy flux U_0 is set to a value that yields a corrosion time of 85,000 years for the highest sulphide concentration in the distribution given in the table HSTest. With the default values as above, this yields a U_0 -value of $1.62 \cdot 10^{-2}$ m/yr, according to Equations (5), (6), (7), (9a) and (10). This corresponds to a q -value higher than q_{lim} , meaning that Equation (7) should be used for Q_{eq} . Ten lines of output should be generated, with failure times ranging from 85,000 years to 94,000 years in increments of 1,000 years.

5.4 Data row 3: Testing the erosion calculation

The third data row has the same U_0 -value as the first row meaning that the generated corrosion times should be the same. This row also has a value of the fracture aperture, δ , chosen so that the time to reach advective conditions is 50,000 years. With the given U_0 -value and the default parameter values

$$\begin{aligned} A_{ero} &= 27.211 \\ m_{buffadv} &= 1200 \text{ kg} \\ f_{dilute} &= 0.25 \end{aligned}$$

and otherwise default parameters as above, the δ -value obtained with Equation (2) solved for δ combined with Equations (1) and (3) is $2.33 \cdot 10^{-3}$ m. The ten generated failure times should thus be 900,000 years, 910,000 years etc up to 990,000 years.

5.5 Data rows >3: Further testing of the generation of result tables and of rejection criteria

The fourth data row is identical to the third, but with a δ -value of $7.20 \cdot 10^{-4}$ m to generate a time to reach advective conditions of 100,000 years. This means that only five data points out of ten in the table of sulphide concentrations give valid corrosion times with the SR-Site default settings. Hence only five failure times should be generated ranging from 950,000 years to 990,000 years.

The test file contains 6008 rows of data. All rows beyond data row 4 have U_0 -values of zero meaning that they should not generate any failure times. Eight lines have data such that the corresponding deposition positions should be rejected with the SR-Site default settings:

- Row 12 according to the FPC criterion
- Rows 13 through 17 according to the EFPC criterion
- Row 18 according to the fracture length criterion
- Row 19 according to the combined T/L-criterion

Rows 20 through 25 have data such that they should just escape fulfilling the rejection criteria. Remaining rows should not result in rejection according to any of the criteria.

5.6 Expected results of a test run

Running of the model with the TestCaseHydro.xlsx and the SR-Site default settings should thus result in the generation of 35 failure times with 10 related to each of deposition position IDs 1, 2 and 3, and 5 to position ID 4 in sheet "InputTrptCalcs". The values of FProb and TwProb in this sheet should be the same as F and TW, respectively, for the corresponding position IDs in TestCaseHydro.xlsx (column A).

The test run should also result in the following key outputs; cells C25 – C36 in sheet “Info”:

- Mean number of failed canisters at 1,000,000 years: 3.5 (1 from each of data rows 1-3; 0.5 from data row 4)
- Mean number of failed canisters at 1,000,000 years, corrected: 3.5 (1 from each of data rows 1-3; 0.5 from data row 4)
- Number of failed canisters at 1,000,000 years for highest sulphide concentration: 4 (data rows 1-4)
- Mean number of failed canisters at 100,000 years, corrected: 1 (from data row 2)
- Earliest failure time: 85,000 years (from data row 2)
- Total number of positions: 6008 (total number of data rows in TestCaseHydro.xlsx)
- Number of rejected positions: 8 (from data rows 11-18)
- Number of advective positions at 1,000,000 years: 4 (data rows 1-4)
- Number of advective positions at 100,000 years: 3 (data rows 1-3)
- Earliest advective time: 0 (data rows 1 and 2)
- Any edge positions: No
- Check sum: 0 (indicating that resulting number of failure times is correct in sheet "Calc")

6 Recommended developments

6.1 Correcting the implementation of Equation (9)

The erroneous implementation of Equation (9) should be corrected. This is readily achieved by correcting the formula for “DiffConst” in cell C52 in sheet “Info”. In the code documentation (this document) Equation (9a), the text relating to it in section 3.2 and Appendix 1 should be deleted. The numbering of the remaining Appendices should be adjusted.

This also means that the test case has to be changed according to the following.

- In section 5.2 (of this document), the value of q_{lim} should be $0.08845 \text{ m}^3/\text{yr}$ and the corresponding to U_θ -value should be $5.05 \cdot 10^{-3} \text{ m/yr}$.
- In section 5.3 (of this document), the U_θ -value should be $1.28 \cdot 10^{-2} \text{ m/yr}$, and the reference in the text should be to Equation (9), instead of (9a).
- The corresponding changes of U_θ should be made in the test input file “TestCaseHydro.xlsx”.

6.2 Differentiating between the variables w and h_{can}

The variable w , introduced in the text relating to Equation (3) should be implemented as a separate variable in the model rather than being identical with the variable h_{can} . It needs to be defined in sheet “Info” and implemented in columns R, S, U, AV and BH in sheet “Calc” where it should replace the variable h_{can} .

This is readily achieved by changing the existing global variable name h_{can} , defined in cell C48 in sheet “Info”, to w with Excel’s name editor (which automatically updates the names in the formulae of all cells of the mentioned columns) and then introducing a new global variable h_{can} in sheet “Info” and changing the variable w in cell C62 back to h_{can} .

The text relating to Equation (3) should also be updated.

Appendix 1. Equation (9) vs Equation (9a)

As described in section 3.2, an erroneous version of Equation (9), described by Equation (9a), was implemented in all versions of the code up to and including v 1.0.

In the following, it is demonstrated that Equation (9a) gives *i*) a slightly lower probability of canister failure due to corrosion and, as a consequence, *ii*) slightly lower calculated doses than Equation (9).

Extent of corrosion

Table 1 shows the calculated mean number of failed canisters at one million years after repository closure using both Equation (9a) and Equation (9). The cases are the same as those summarised in Figure 12-18 of the SR-Site main report, TR11-01 Vol III, p. 609. As seen in the table, the calculated extent of canister corrosion in SR-Site is slightly higher compared to that obtained with the correct Equation (9).

Table 1. Mean number of failed canisters for a number of corrosion cases calculated in SR-Site. The values in column "Equation (9a)" are those reported in the SR-Site main report, TR-11-01 Vol III, p. 609, Figure 12-18.

Case	Equation (9a); used in SR-Site	Using Equation (9)
Uncorrelated hydrogeological DFN model Initial advection in all deposition holes	1.2	1.06
Uncorrelated hydrogeological DFN model SR-Site erosion model	0.65	0.57
Semicorrelated hydrogeological DFN model Initial advection in all deposition holes	0.18	0.13
Semicorrelated hydrogeological DFN model SR-Site erosion model	0.12	0.079
Fully correlated hydrogeological DFN model Initial advection in all deposition holes	0.86	0.73
Fully correlated hydrogeological DFN model SR-Site erosion model	0.57	0.47

Dose consequences

The dose consequences for the above corrosion cases have been calculated using the analytical radionuclide transport models described in section 13.4.4 of the SR-Site main report TR-11-01. In section 13.5.10 of TR-11-01 it is demonstrated that the analytical models yield results very similar to those obtained with the more detailed but also considerably more computationally demanding numerical models.

Figure 1 is taken from the SR-Site main report (Figure 13-42, p. 689 in TR-11-01) and shows the results of dose consequence calculations of the six corrosion cases in Table 1 above. These are also the corrosion cases considered in the risk summation and the compliance demonstration in SR-Site, as discussed in section 13.9, p. 724ff in TR-11-01 Vol III. Figure 2 shows results of the same calculation cases as in Figure 1, but using Equation (9) when determining the canister failure times.

As seen when comparing the two Figures, the use of Equation (9) yields marginally lower doses and marginally later onset of radionuclide releases compared to results obtained with Equation (9a).

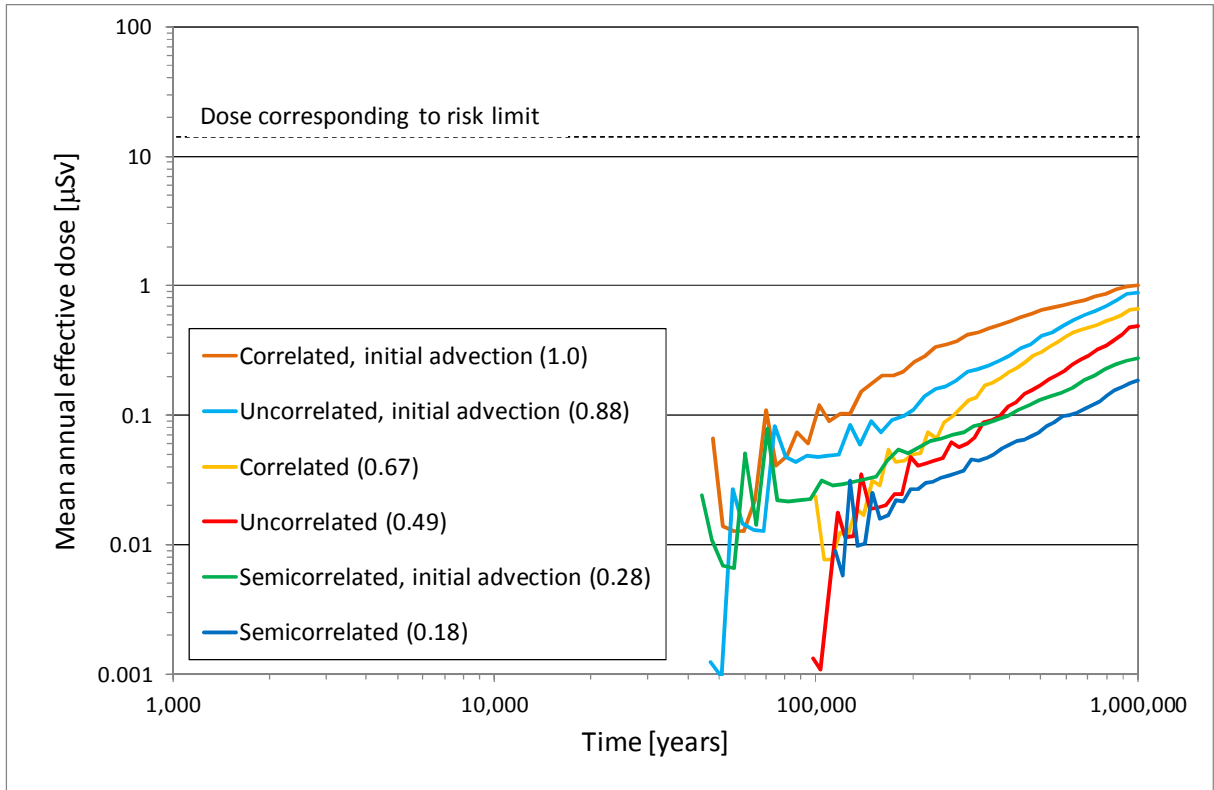


Figure 1. Far-field mean annual doses for analytical, probabilistic calculations of the six corrosion variants of the corrosion scenario, i.e. the six cases in Table 1 when using Equation (9a). The peak doses are given in parentheses in μSv . (Figure 13-42, p. 689 in TR-11-01.)

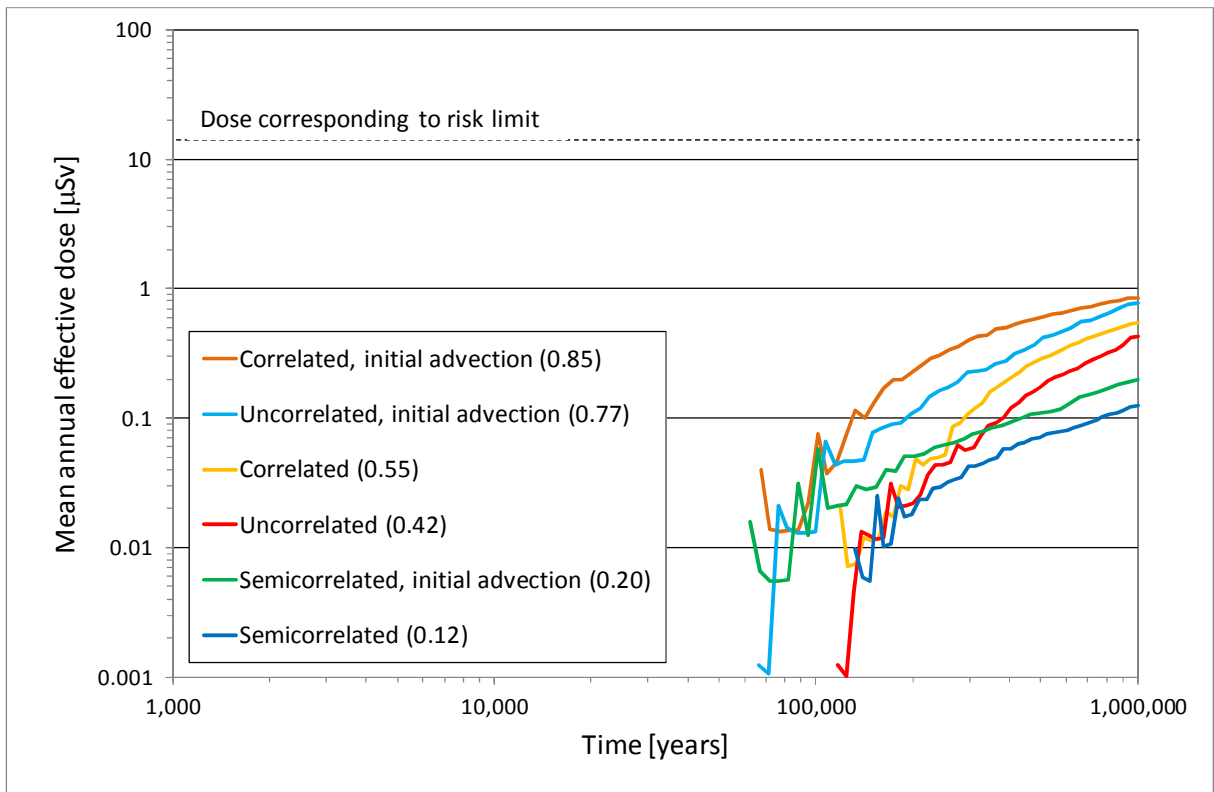


Figure 2. The same calculation cases as in Figure 1, but using Equation (9) when determining the canister failure times.

Conclusion

It is concluded that the use of the erroneous Equation (9a) in the SR-Site calculations gives *i*) a slightly too high probability of canister failure due to corrosion and, as a consequence, *ii*) slightly higher calculated doses than when using the correct Equation (9). No conclusions drawn in the SR-Site main report are, therefore, affected by this error.

Storage of results

The results of the above calculation cases are stored under ID 1265612 (times of failure due to corrosion) and ID 1260107 (radionuclide transport calculations) in SKB's document management system SKBdoc.

Appendix 2. Diffusion through an intact buffer with spalling in the deposition hole

The corrosion rate for the case with diffusion through an intact buffer and where the corroding agent (sulphide) is provided from the flowing groundwater in a fracture intersecting a deposition hole affected by spalling is given in Equation 4-19a in TR-10-66:

$$v_{corr}^{spalling} = Q_{eq} \cdot [HS^-] \frac{f_{HS} \cdot M_{Cu}}{W_{zone} \cdot L_{zone} \cdot \rho_{Cu}}$$

where all variables are explained in sections 4.2.1 and 4.2.2 of TR-10-66. All input data except the sulphide concentration and Q_{eq} are given in Appendix 1 to TR-10-66. The sulphide concentration was 10^{-5} M and the hydrogeological Q_{eq} -values were taken from results obtained with the base case of the semi-correlated hydrogeological DFN model. However, as mentioned in section 4.6.5 above, in versions of the code up to v 0.9, and hence in the calculations reported in SR-Site, a now obsolete, slightly more pessimistic expression was used:

$$v_{corr}^{spalling} = [HS^-] \frac{f_{HS} \cdot M_{Cu}}{\rho_{Cu}} \frac{1}{\frac{2\pi r_{Can} h_{Can}}{(Q_{eqhydro} + Q_{eqspalling}) \cdot BCF} + \frac{d_{buffer}}{D_{e,buffer}}}}$$

where again all variables are explained in sections 4.2.1 and 4.2.2 of TR-10-66 and where data were obtained from the sources described above.

Results of calculation cases using the two expressions are shown in Figure 1 (Equation 4-19a in TR-10-66) and in Figure 2 (old expression). As seen by comparing the Figures, the results obtained with the two expressions are virtually indistinguishable. The old expression is slightly more pessimistic, yielding slightly higher corrosion rates.

It is concluded that the use of the old expression in the SR-Site calculations yield results virtually indistinguishable from those obtained with the established Equation 19a in TR-10-66 when determining corrosion rates for diffusive conditions in deposition holes affected by thermally induced spalling, and that none of the conclusions in the safety assessment SR-Site are affected by the unintentional use of the old expression.

Storage of results

The results of the above calculation cases are embedded in the model files "ErosionCorrosionModel_1_0.xlsx" (use of Equation 9a in TR-10-66) and "ErosionCorrosionModel_0_8.xlsx" (use of obsolete expression); the relevant result plots appear in sheets "CorrDiffPlt" in the files. Both files are stored under ID 1265612 in SKB's document management system SKBdoc.

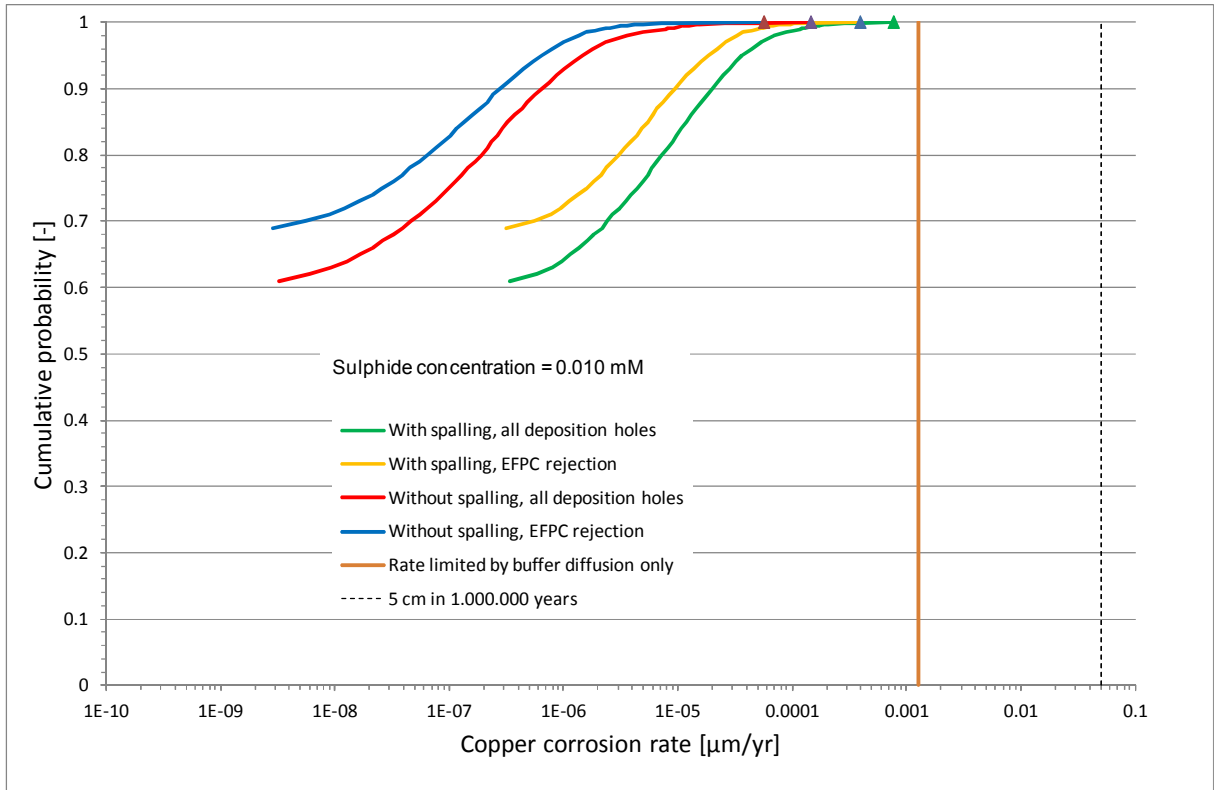


Figure 1. Corrosion rates calculated using Equation 4-19a in TR-10-66.

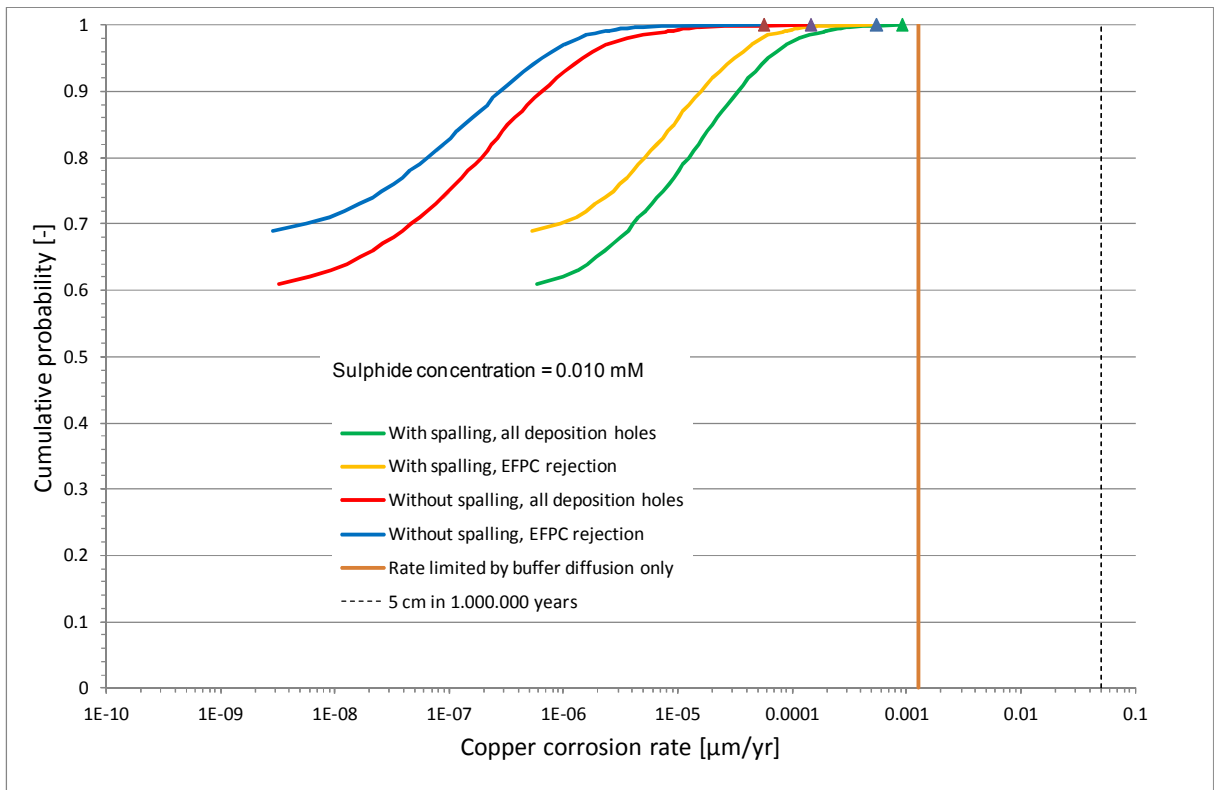


Figure 2. Corrosion rates calculated using obsolete expression given in text above.

Appendix 3. Corrosion caused by oxygen penetrating to the repository for advective conditions in the deposition hole

This Appendix documents calculations of oxygen penetrating to the repository for advective conditions in the deposition hole. The prerequisites of the modelling and the results are reported in section 12.6.2 of TR-11-01, subsection “Oxygen penetration”, p. 603ff.

This calculation was done using a dedicated version of v 0.8 of the erosion/corrosion model, with relevant alterations of parameter values. These alterations are all marked in red in the sheet “Info” in the file “ErosionCorrosionModel_0_8_Oxygen.xlsx”.

Oxygen concentrations for each deposition hole were obtained from a separate calculation, where the resulting oxygen concentrations are given in column A of sheet “Real_F_values_NotSorted” in file “O2-New_Equation.xlsx”. These values were transferred to column CX in sheet “Calc” of file “ErosionCorrosionModel_0_8_Oxygen.xlsx”.

Hydrogeological data for the calculations of both oxygen concentrations and corrosion were obtained from the case “fs_nocpm_Q1_glacial_III”. These data appear in the sheet with the same name in “ErosionCorrosionModel_0_8_Oxygen.xlsx”. This was found to be the hydrogeological case most favourable for oxygen penetration, see further section 12.6.2 of TR-11-01, subsection “Oxygen penetration”, p. 603ff.

The corrosion calculations are carried out in column CZ in sheet “Calc” of “ErosionCorrosionModel_0_8_Oxygen.xlsx”, using the expressions given section 3.2 above, but with data relevant for oxygen as the corroding agent. The calculated corrosion rates are post processed in columns DA, DE and DF and a plot of the results is given in sheet “CorrOxPlt” of “ErosionCorrosionModel_0_8_Oxygen.xlsx”.

The model file “ErosionCorrosionModel_0_8_Oxygen.xlsx” is stored under ID 1265612 in SKB’s document management system SKBdoc.

The file “O2-New_Equation.xlsx” containing the oxygen concentrations is stored under ID 1265689.