Assessment of complexing agent concentrations in SFR

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March 2014

SKB

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Abstract

Low- and intermediate-level radioactive waste produced in Sweden is deposited in the Repository for Short-Lived Low- and Intermediate-Level Waste (SFR). Complexing agents used at the nuclear sites are present in this waste and others will be generated in situ through the degradation of waste components such as cellulose. These may potentially affect the safety function of the BMA, Silo and BTF vaults of SFR by reducing radionuclide sorption and enhancing radionuclide transport to the geosphere. This report therefore updates a previous assessment of complexing agents in SFR (Fanger et al. 2001). First, the literature is reviewed to a) identify the materials that are likely to degrade and produce complexing agents in situ, b) obtain data for the likely rates of relevant processes, and c) assess complexing agent and degradation product sorption to hydrated cement and their likely solubility and stability under repository conditions, to optimise the later calculations. The mass of different complexing agents and cellulose in each type of SFR waste package is then summarised using the most recent information from the nuclear sites and the new Waste Inventory Report (SKB 2013). Finally, the concentrations of complexing agents have been calculated in each relevant waste package type and larger unit of SFR, e.g. 1BMA compartments, 2BMA caissons, the Silo construction and BTF waste zone, as well as each rock vault. In the case of the cellulose degradation product, isosaccharinate (ISA), concentrations were calculated as a function of time. Sorption of ISA and gluconate to hydrated cement has been accounted for, as have the solubility limits of the α-diastereoisomer of ISA and oxalate in a cementitious system. All other complexing agents were assumed to be in solution. The results show that ISA, nitrilotetraacetate (NTA), and citrate will be present at the highest concentrations.

Contents

1   Introduction

Low- and intermediate-level radioactive waste produced in Sweden is deposited in SFR. Complexing agents used at the nuclear sites are therefore present in the wastes and other complexing agents will form in situ, notably isosaccharinate (ISA) during the degradation of cellulose. Organic cement additives may also have complexing properties. Since complexing agents may reduce radionuclide sorption to hydrated cement phases in the repository and enhance migration into the geosphere, it is important to assess the concentrations present in SFR.

A previous study (Fanger et al. 2001) summarized the amounts and concentrations of complexing agents anticipated in SFR. This report updates these estimates, using the most recent waste inventory (SKB 2013), new assessments of detergent use at the nuclear sites and the improved scientific understanding of cellulose degradation processes and gluconate sorption to hydrated cement. The results of this report will provide a basis for the Data Report for the safety assessment SR-PSU (SKB 2014a), and will therefore be included in the safety assessment for radionuclide transport.

2 Literature review

The literature review in this section revisits and updates the literature review in Fanger et al. (2001). The purpose of this section is to identify the complexing agents in SFR for which concentration data are required. The Data Report for the safety assessment SR-PSU (SKB 2014a) provides comprehensive information on the effects of different complexing agents.

2.1 Complexing agents in low- and intermediate-level waste

A wide range of complexing agents are present in low- and intermediate-level radioactive wastes from the detergents and materials used at the nuclear power plants and chemicals used in waste conditioning. Low molecular mass organic complexing agents, such as the decontamination agents EDTA (ethylenediaminetetraacetate), NTA (nitrilotriacetate), citrate, oxalate and gluconate, and degradation products of cellulose are of particular importance for SFR. Cement additives and degradation products of polymers, bitumen, cation-exchange resins and anion-exchange resins may also be relevant.

Inorganic ligands such as CO_3^{2-}, NO_3^-, SO_4^{2-}, S^{2-}, PO_4^{3-}, CN^-, $B(OH)_4^-$, F^-, I^-, Cl^- and Br^- will also be present in the surrounding groundwater and/or the radioactive waste. It has been concluded that, under the high pH conditions of a cementitious repository, only cyanide complexes are of importance for radionuclide (Ni(II), Ag(I), Pb(II)) sorption (Bradbury and Van Loon 1997). However, cyanide present as the hexacyanoferrate anion ($Fe(CN)_6^{4-}$) forms weak complexes with metal cations (Bradbury and Van Loon 1997). Inorganic ligands are not considered further in this report.

2.2 Degradation processes and products

Cellulose, UP2 filter aid, bitumen and ion-exchange resins are the main organic substances that may degrade to produce complexing agents in SFR. The current understanding of their degradation processes is described in Sections 2.2.1–2.2.4.

2.2.1 Cellulose

Degradation mechanisms

Substantial amounts of cellulosic materials such as paper, textiles and wood are often present in low- and intermediate-level radioactive wastes. Under the highly alkaline conditions of a cementitious repository, cellulose will degrade to water soluble, low molecular weight compounds. The mechanisms and rates of alkaline cellulose degradation have been investigated in a number of studies (e.g. Glaus and Van Loon 2008, Pavasars 1999, Van Loon and Glaus 1998, Bradbury and Van Loon 1997).

Cellulose degrades through the "peeling off" reaction under alkaline conditions. In this reaction, reducing end groups of the cellulose polysaccharide chain isomerise into reactive interim products that are then eliminated from the chain (Van Loon and Glaus 1998). The reaction produces new reducing end groups for further reaction, leading to step-wise elimination of glucose units and depolymerisation of the chain. The reaction sequence stops when the reactive interim product is converted to a stable meta-saccharinic end group on the polysaccharide chain, or a crystalline (inaccessible) region of the chain is reached. These two stopping reactions are termed the chemical stopping reaction and the physical stopping reaction, respectively. Once all end groups are stable or inaccessible, the peeling off reaction depends on the formation, or increased accessibility, of reducing end groups. The possible reaction mechanisms for this are termed "mid-chain scission", which involves alkaline hydrolysis of glycosidic bonds in the polymeric chain, and "decelerated peeling", which involves a dynamic equilibrium between crystalline and amorphous structures of cellulose (Glaus and Van Loon 2008).

Degradation products

The products of alkaline cellulose degradation depend on the composition of the surrounding solution (Bradbury and Van Loon 1997, Van Loon and Glaus 1997). In the presence of Ca^{2+}, as found in cement pore waters, the formation of ISA is favoured with a typical yield of ~80% (Bradbury and Van Loon 1997, Van Loon and Glaus 1997, Pavasars et al. 2003, Glaus and Van Loon 2008). The α- and β-diastereoisomers of ISA are formed in approximately equal proportions (Van Loon et al. 1999a). α-ISA exhibits strong complexing properties and therefore is of concern in terms of its potential to enhance radionuclide mobility (Pavasars 1999, Glaus et al. 1999, Van Loon et al. 1999b). Minor degradation products comprise short chain aliphatic carboxylates such as formate, acetate and lactate (Glaus et al. 1999, Van Loon et al. 1999a).

Degradation rates

Cellulose degradation rates reported in the literature vary according to the cellulosic material and experimental conditions used. Different types of cellulose are polymerised to different degrees and this affects the mole fraction of reducing end groups initially present in the material, i.e. available for reaction. Also, the pH, cations present, temperature and redox conditions are important (Pavasars 1999, Van Loon and Glaus 1997, Glaus and Van Loon 2009).

The majority of experiments have been performed for a limited period of time or at high temperatures, and extrapolation of the results to repository conditions and timescales has generated contrasting conclusions. However, Glaus and Van Loon (2008) studied the degradation of four cellulosic materials under artificial cement porewater conditions over a 12 year period, the longest study to date. Their data for Tela tissue degradation are therefore considered here to be the most relevant and complete data for predicting cellulose degradation in SFR, and are applied throughout this report. Glaus and Van Loon (2008) presented two equations to describe cellulose degradation, the first using mid-chain scission to control the long-term degradation rate and the second using decelerated peeling. They argued that decelerated peeling is the more likely mechanism, however, the equation for this process does not extrapolate to the timescales of interest here, while the equation involving midchain scission does. Therefore, the equation for the mid-chain scission reaction (Glaus and Van Loon 2008; shown here as Equation 2-1) has been used to estimate the degree of cellulose degradation over time.

$$(celdeg)_t = 1 + e^{-k_h t}\left[\frac{k_1}{k_t}\cdot(G_r)_0\cdot\left(1-e^{-k_t t}\right)-1\right]$$
<div align="right">Equation 2-1</div>

where

$(celdeg)_t$ = fraction of cellulose degraded as a function of time

k_h = product of the average number of peeled glucose units and the intrinsic reaction rate constant for the mid-chain scission reaction

k_1 = first order rate constant for the propagation of the peeling off reaction

k_t = first order rate constant for the stopping reaction

$(Gr)_0$ = initial mole fraction of reducing end groups

Glaus and Van Loon (2008) determined the following reaction rate constants for Tela tissue degradation by best fit to their experimental data:

$k_h = (1.0 \pm 0.2)\cdot 10^{-7}\ h^{-1}$

$k_1 = (1.0 \pm 0.1)\cdot 10^{-2}\ h^{-1}$

$k_t = (2.9 \pm 0.5)\cdot 10^{-4}\ h^{-1}$

The degree of polymerisation of a material has an inverse relationship with the initial mole fraction of reducing end groups $((Gr)_0)$, and this generated a $(Gr)_0$ value of $9.0\cdot 10^{-4}$ for Tela tissue.

The experimental data showed a rapid initial degradation rate and >3% of the cellulose in Tela tissue degraded over the first 2 years. The remaining cellulose then degraded more slowly; Equation 2-1 calculates that cellulose degradation will be virtually complete (~99%) after 5,000 years. Similarly,

using the rate constants and $(Gr)_0$ values given in Glaus and Van Loon (2008) for paper, the cellulose in paper will be almost completely degraded (~100%) after 5,000 years. The experimental data and associated constants derived for cotton, suggest that cotton degradation will be slower, with ~76% degraded after 5,000 years, and ~99% after 25,000 years.

Previous SFR reports have estimated ISA concentrations based on the degradation of 1.8% of the cellulose present (Skagius et al. 1999, Fanger et al. 2001), although Fanger et al. (2001) also calculated the concentrations arising from 2.6 and 10% degradation. The work of Glaus and Van Loon (2008) suggests that these assessments underestimate the potential ISA concentrations significantly.

2.2.2 UP2 filter aid

UP2 filter aid consists of polyacrylonitrile fibres with a chemical formula of $[C_3H_3N]_n$. The structure has been shown to undergo relatively small changes in an experiment simulating its use at a nuclear site, altering from an isotactic to syndiotactic structure (Duro et al. 2012). During alkaline degradation, nitrile groups are slowly hydrolysed to amides and carboxylic acids (e.g. Ermakov et al. 2000), with carboxylic acids being the likely final product. Depolymerisation or other reactions generating low molecular units will also take place; Duro et al. (2012) found that soluble UP2 degradation products were a mixture of carboxylic acids, amides, alkenes and ketones. However, only a limited proportion of the degradation products were characterized in this study (8 and 28% at pH 12.5 and 13.4, respectively).

The rate of UP2 degradation has been investigated under alkaline conditions in three studies (Dario et al. 2004, Duro et al. 2012, Holgersson et al. 2011). Temperature and pH had a very clear influence on the rate of degradation and the lowest rates of degradation were found at pH 12.5 compared to pH 13.4, and room temperature compared to 60°C. Duro et al. (2012) degraded UP2 fibre mass at pH 12.5 (buffered by $Ca(OH)_2$) and room temperature and found that the DOC concentration initially increased rapidly and then reached a plateau after about 300 days.

UP2 will be conditioned in bitumen (F.17 type waste) prior to disposal, which is likely to delay the onset of alkaline degradation for some time. Therefore, degradation is expected to take place at pH 12.5 (portlandite buffered conditions) or less and the available evidence (Duro et al. 2012) suggests that this will limit degradation.

2.2.3 Bitumen

Bitumen is a mixture of high molecular aliphatic and aromatic hydrocarbons, including components such as nitrogen, oxygen and sulphur (Allard et al. 1985). It is therefore expected to change chemically over time under oxidising conditions, including via microbial degradation. However, according to the Waste form and packaging process report for the safety assessment SR-PSU (SKB 2014c), microbial degradation of bitumen will be very slow under anaerobic, low flow and high pH conditions. These conditions will prevail for a considerable period of time in the long-term safety analysis.

The chemical products of bitumen degradation under oxic conditions are reported to have weak or negligible complexing power and will have no significant influence on the sorption of radionuclides onto cementitious materials (Pettersson and Elert 2001). The dissolved concentrations of organic substances and trace elements were not found to be elevated in the alkaline groundwater from a site in northern Jordan with natural occurring bitumen (SKB 1991).

2.2.4 Ion-exchange resins

Ion-exchange resins used at the Swedish nuclear sites consist of polystyrene chains with amine functional groups in anion exchangers and sulfonic acids in cation exchangers (Allard et al. 1985). Low sulfur cation exchange resins are also used, which have carboxylate functional groups on a polyacrylate support (Allard et al. 2002). Radiolytic degradation of cation- and anion-exchange resins produces oxalate (Van Loon and Hummel 1999a) and amines (Van Loon and Hummel 1999b), respectively, among the degradation products. However, chemical degradation was not observed in these studies and radiolytic degradation is not expected to be significant given the relatively low radioactivity associated with SFR wastes. In any case, radiolytic degradation products have been shown to have a negligible influence on the sorption of radionuclides to cementitious materials (Bradbury and Sarott 1994, Bradbury and Van Loon 1997, Allard et al. 1985).

2.3 Behaviour and impact of complexing agents

Complexing agents only affect the safety of a low- or intermediate-level waste repository if they are stable, dissolved and able to affect the sorption of radionuclides under the prevailing geochemical conditions. These issues are reviewed in this section for the degradation products identified in Section 2.2, common decontamination agents (i.e. EDTA, NTA, citrate, oxalate and gluconate) and organic cement additives. Note that gluconate is not used as a cement additive in SFR.

2.3.1 Degradation of complexing agents, precipitation and sorption to hydrated cement

Although most complexing agents undergo chemical or biological degradation under aerobic conditions, their degradation under anaerobic, highly alkaline conditions is less well defined. ISA degradation has, however, been studied in a suite of relevant long-term (hundreds of days) experiments (Glaus and Van Loon 2009). Within the experimental errors, there was no evidence to suggest that ISA degraded under conditions representative of a cementitious repository (Glaus and Van Loon 2009). This is consistent with the results of cellulose degradation experiments in which ISA was present at a constant proportion of the total dissolved organic carbon under artificial cement porewater conditions over a period of 12 years (Glaus and Van Loon 2008). Significant microbial degradation of ISA is not expected in repository environment until late stages of cement degradation, because a high pH (> 12) limits microbial processes, including ISA degradation by alkaliphilic bacteria (Rizoulis et al. 2012). Therefore, for this report, ISA degradation has not been considered. Since the degradation of other complexing agents has not been demonstrated under repository conditions, they are also assumed to be stable for the purposes of this report.

The dissolved concentrations of complexing agents may also be affected by precipitation and/or sorption to available hydrated cement. Precipitation is important for both oxalate and the α-diastereoisomer of ISA in a cementitious repository, due to their relatively low solubility products with Ca^{2+}. Oxalate concentrations are expected to be limited to $\leq 10^{-5}$ M (Van Loon and Hummel 1995), while dissolved α-ISA concentrations have been calculated to be limited to 0.02 M during the portlandite phase of cement degradation (0.02 M Ca^{2+}; 0.05 M ionic strength) (Van Loon and Glaus 1998). The α-diastereoisomer of ISA has the greater ability to complex radionuclides (Pavasars 1999, Glaus et al. 1999, Van Loon et al. 1999b) and therefore the solubility of this isomer is most relevant.

Sorption of ISA and gluconate to hydrated cement has been well characterised for the early stages of cement degradation, and the sorption isotherms can be used to estimate solution phase concentrations of these complexing agents in a repository. Experiments have shown that hydrated cement can sorb up to 0.3 mole kg^{-1} of ISA (Van Loon et al. 1997, Van Loon and Glaus 1998) or 0.74 mole kg^{-1} gluconate (Glaus et al. 2006).

Van Loon et al. (1997) presented two different sorption isotherms for estimating the sorption of ISA to hydrated cement (Equation 2-2 and Equation 2-3). The non-linear two-site model (Equation 2-3) was found to be the better isotherm for ISA (Van Loon et al. 1997). α- and β-ISA show comparable sorption isotherms (Van Loon and Glaus 1998).

$$[ISA]_{sorbed} = \frac{K \cdot q \cdot (ISA)_{eq}}{1 + K \cdot (ISA)_{eq}}$$

Equation 2-2

where

$[ISA]_{sorbed}$ = sorbed concentration of ISA at equilibrium (mol kg^{-1})

K = adsorption-affinity constant = 286 L mol^{-1}

q = adsorption capacity of the hydrated cement for ISA = 0.17 mol kg^{-1}

$(ISA)_{eq}$ = solution phase concentration of ISA at equilibrium (M)

$$[ISA]_{sorbed} = \frac{K_1 \cdot q_1 \cdot (ISA)_{eq}}{1 + K_1 \cdot (ISA)_{eq}} + \frac{K_2 \cdot q_2 \cdot (ISA)_{eq}}{1 + K_2 \cdot (ISA)_{eq}}$$

Equation 2-3

where

K_1 = adsorption-affinity constant of site 1 = 1,730 L mol^{-1}

q_1 = adsorption capacity of site 1 = 0.1 mol kg^{-1}

K_2 = adsorption-affinity constant of site 2 = 12 L mol^{-1}

q_2 = adsorption capacity of site 2 = 0.17 mol kg^{-1}

Gluconate sorption is also described by Equation 2-3, with

$K_1 = (2 \pm 1) \cdot 10^6$ L mol^{-1}

$q_1 = 0.04 \pm 0.02$ mol kg^{-1}

$K_2 = (2.6 \pm 1.1) \cdot 10^3$ L mol^{-1}

$q_2 = 0.7 \pm 0.3$ mol kg^{-1} (Glaus et al. 2006)

The sorption of other complexing agents to hydrated cement has not been studied to the same degree, and sorption isotherms are not available. Sorption of all complexing agents other than ISA and gluconate is therefore assumed to be zero in this report. There is, however, evidence that EDTA shows an affinity for degraded cement (Pointeau et al. 2008), and that NTA and citrate may show some affinity for hydrated cement (Dario et al. 2004).

2.3.2　Impact of complexing agents on radionuclide solubility and sorption

This section provides an overview of results from experimental and theoretical studies investigating the impact of complexing agents on the solubility of radionuclides and radionuclide sorption to relevant solid phases. The individual references have not been evaluated in detail.

Impact of ISA on radionuclide solubility

ISA is known to enhance the solubility of tri, tetravalent and, to a lesser extent, divalent ions. At pH 12, the solubility of Pu(IV) has been found to increase significantly with ISA concentrations above $1 \cdot 10^{-5}$ M; changing the ISA concentrations from $1 \cdot 10^{-3}$ to $5 \cdot 10^{-3}$ M increased the solubility of Pu from ~10^{-5} to ~10^{-4} M (Greenfield et al. 1997). An ISA concentration of $2 \cdot 10^{-3}$ M has also been found to increase the solubility of U(IV), Th(IV) and Pu(IV) by factors of 250, 500 and $2 \cdot 10^5$ respectively (Allard et al. 1995).

Other experiments have shown that ISA interacts with Ni(II) (Warwick et al. 2003) and U(IV) (Warwick et al. 2004). The log stability constant derived for U(IV)(OH)$_4$ISA, of 49 ± 2, suggests that this complex has a high stability (Warwick et al. 2004).

Impact of ISA on radionuclide sorption

Sorption of ISA onto hydrated cement will affect its ability to enhance radionuclide solubility (Holgersson 2000) and experimental results are therefore influenced by the solid/solution ratio of the experiment, as well as the solid phase used. Therefore, comparability between experimental results is only expected if the same solid/solution ratio was applied or the concentration of ISA remaining in the solution phase was reported. Van Loon and Glaus (1998) used feldspar specifically to avoid the complications of ISA sorption to the experimental solid phase. Furthermore, whether total ISA or α-ISA is used may affect the impact on radionuclide sorption. Van Loon and Glaus (1998) investigated the effect of α- and β-ISA on Eu(III) sorption individually, and found that the α-ISA complex was approximately 100 times more stable than the equivalent β-ISA complex. However, since α-ISA comprises approximately half of the total ISA, the potential variations due to experimental setup exceed the variations due to this. Therefore, the discussion below does not specify whether ISA or α-ISA was used in each experiment. It is also worth noting that different experimental approaches, such as the order in which the ligand and metal are added and the times between these, may affect short term results due to kinetics (e.g. Reinoso-Maset et al. 2012).

The effect of ISA on Eu(III) sorption has been investigated in a number of studies. Van Loon and Glaus (1998) found that ISA concentrations $>1\cdot10^{-4}$ M affected Eu(III) sorption to feldspar in artificial cement porewater. Dario et al. (2004) found that short term (24 hours) Eu(III) sorption to hydrated cement was reduced when ISA was added at concentrations of 10^{-3} and 10^{-2} M. Changes over 400 days were investigated using $10^{-2.5}$ M ISA and although Eu(III) sorption increased during the first 50 days, ISA reduced the sorption of Eu(III) at equilibrium by over an order of magnitude. Wieland et al. (1998) found that ISA had a negligible effect on Eu(III) sorption to hydrated cement until the ISA concentration exceeded 10^{-2} M. Europium sorption on hardened cement paste was reduced by a factor 100 at equilibrium concentrations of $\sim10^{-1}$ M ISA (Bradbury and Van Loon 1997).

ISA was found to reduce Th(IV) sorption to hardened cement paste by over four orders of magnitude as the ISA equilibrium concentrations increased from 10^{-4}–10^{-2} M, but it had no influence at concentrations $\leq10^{-4}$ M (Bradbury and Van Loon 1997, Wieland et al. 1998). Van Loon and Glaus (1998) found that ISA concentrations in the range 10^{-4}–10^{-3} M reduced Th(IV) sorption to feldspar. Experiments by Pavasars (1999) showed that the addition of a high concentration of ISA ($3\cdot10^{-2}$ M) resulted in a persistent reduction of radionuclide sorption; after 3 months Th(IV) sorption was reduced at least 50 times. However, lower concentrations ($3\cdot10^{-3}$–0^{-3} M ISA) only reduced sorption of ^{234}Th(IV) significantly for 1 month (Pavasars 1999).

ISA has also been found to reduce Ni(II) sorption to feldspar, but significant effects were only seen at ISA concentrations higher than 10^{-2} M (Van Loon and Glaus 1998). The degradation products of cellulosic materials (tissues, cotton and paper) were more effective at solubilising Ni(II), but these have not been fully characterised or studied to the same extent as ISA (Van Loon and Glaus 1998, Van Loon et al. 1999b).

The sorption of anionic species may also be reduced by the presence of ISA through competition for surface binding sites. Sorption of SeO_3^{2-} to un-degraded (pH 13.3) and degraded (pH 12.0) hardened cement paste was reduced by a factor of two by the addition of $2\cdot10^{-3}$ and $5\cdot10^{-4}$ M ISA, respectively (Pointeau et al. 2008).

Impact of UP2 filter aid degradation products

Duro et al. (2012) investigated the effect of UP2 degradation products on the sorption of ^{152}Eu to cement. The degradation products obtained at pH 12.5 (buffered by $Ca(OH)_2$) and room temperature, which are the most relevant to SFR, did not affect Eu sorption significantly. The maximum degradation product concentration in this experiment was equal to the maximum concentration obtained in the associated degradation experiments, after which degradation ceased, and was approximately 8 mg L^{-1} DOC. The degradation experiments used an initial UP2 fibre concentration of 25 g L^{-1}, which is equivalent to the highest UP2 fibre concentration currently disposed in 1BMA (in compartment 6). Therefore, the data are very relevant to SFR and indicate that radionuclide mobility will not be affected significantly by UP2 degradation.

Although degradation products formed under different pH (13.4) and/or temperature (60°C) conditions have been found to affect long-term Eu sorption at DOC concentrations of 11–36 mg L^{-1} (Dario et al. 2004, Duro et al. 2012), these studies are not considered to be of equal relevance to SFR. UP2 is therefore not considered further in this report.

Impact of gluconate

Experiments have shown that gluconate interacts with Ni(II) (Warwick et al. 2003) and U(IV) (Warwick et al. 2004). The log stability constant derived for $U(IV)(OH)_4GLU$, of 50 ± 1 suggests that this complex has a high stability.

The effect of gluconate on radionuclide sorption has been studied to a lesser extent than ISA, and with a particular focus on Eu sorption. Gluconate was found to reduce Eu sorption to hydrated cement by approximately three orders of magnitude at gluconate concentrations above 10^{-4} M (Nordén and Allard 1994), however, the Eu concentrations recovered to their original values within approximately 200 days. More recently, Dario et al. (2004) found that 10^{-5}–10^{-4} M gluconate decreased Eu sorption to hydrated cement by up to 4 orders of magnitude after 24 hours. With $10^{-4.5}$ M gluconate, this was followed by rapid on-going sorption of Eu(III) over the following days resulting in a negligible long-term effect.

Here, as with ISA, sorption of the organic complexing agent makes the results particularly sensitive to the experimental set-up.

Impact of other complexing agents

The most important complexing agents used at Swedish nuclear power plants are citrate, oxalate, NTA (and its derivatives), EDTA and gluconate. The ability of these complexing agents to form complexes with radionuclides is affected by the high pH conditions and high Ca^{2+} concentrations of a cementitious repository, due to the stability of radionuclide hydroxy species and Ca^{2+}-organic complexes. Therefore, speciation calculations for Swiss cementitious repository scenarios (pH = 11–13, Ca^{2+} concentration = 0.001–0.1 M) suggested that Ni(II), Mn(II) and Pb(II) would be the only radionuclides to be complexed and that EDTA would be the only complexing agent of significance (Hummel 1993, cited in Bradbury and Sarott 1994). A reduction in the sorption of Ni(II) and Mn(II) was calculated when the EDTA concentration exceeded 10^{-4} M, and the sorption of Pb may be reduced if the EDTA concentration exceeds 10^{-3} M. In the absence of experimental data, Bradbury and Van Loon (1997) selected a hydrated cement sorption reduction factor of 50 for Ni(II) and its chemical analogues when the porewater concentration was $4.6 \cdot 10^{-2}$ M EDTA. Since Pb(II) forms weaker complexes with EDTA, a sorption reduction factor of 5 was used.

Experimental data have also shown that EDTA can have a temporary effect on radionuclide sorption. For example, sorption of Am(III) to hydrated cement was initially reduced by an EDTA concentration of $1.5 \cdot 10^{-3}$ M (Allard and Andersson 1987), but after a period of weeks to months, sorption increased to a point that the EDTA no longer affected the Am(III) concentration. Sorption was much slower with $3 \cdot 10^{-2}$ M EDTA but, after one year, the Am(III) concentration was the same as in the absence of EDTA.

More recent experiments have shown that EDTA, NTA and citrate reduce Eu(III) sorption to hydrated cement at concentrations $\geq 10^{-3}$ M in the short term (24 hours) (Dario et al. 2004). The variation over 400 days was also investigated using EDTA, NTA and citrate concentrations of 10^{-2} M. Eu(III) sorption continued to reach or approach equilibrium by ~100 days. Long-term Eu(III) sorption was reduced by EDTA (4 orders of magnitude), citrate (1–2 orders of magnitude and, to a lesser extent, NTA (>0.5 of an order of magnitude).

The modelling in Hummel (1993, cited in Bradbury and Sarott 1994) shows the importance of concurrent and competing reactions and is a useful demonstration of the complexity of radionuclide-ligand interactions.

Impact of cement additives

Common cement additives include sulphonated naphtalene polymers, lignosulphonates, gluconate, sulphonated melamine polymers, vinyl maleic acid co polymers, and polyether polycarboxylates. Most cement additives have not been found to be of concern in terms of their complexing power. The most common products (e.g. Silix GP and Sika AER) are not strong complexing agents and other cement additives (such as Barra 55, Peramin F and Peramin L) are either relatively weak complexing agents or are only present in small amounts in SFR (Fanger et al. 2001).

However, Sikament 10 which is polymerised from N-vinylamides and derivatives of maleic anhydride, has been found to enhance the solubility of Pu significantly at pH 12.3 (~$5 \cdot 10^{-5}$ M vs 10^{-10} M; McCrohon and Williams 1997), and reduce its sorption to grout (Boult et al. 1998). The sorption experiments showed that Pu did not sorb measurably to grout when the solution phase contained 0.5 or 1% Sikament 10. The authors noted that the amount of Sikament 10 was high, arising from the high solution/solid ratio used, and this may have affected the capacity of the hydrated cement to sorb the additive. Despite this, a further study has shown that solution phase Sikament 10 reduces Eu(III) sorption to hydrated cement (Dario et al. 2004). In this case, it was calculated that in a worst case scenario, defined by hydrated cement with a 3% Sikament 10 content and complete transfer of Sikament 10 to the solution phase, Eu sorption would be reduced by 1 ± 0.5 orders of magnitude. The use of cement additives in SFR will be investigated at a later stage and is not considered further in this report.

3 Complexing agents in SFR

A number of wastes from the Swedish nuclear sites contain cellulose and organic complexing agents. Fanger et al. (2001) reviewed the chemicals present in SFR 1 and identified those that are complexing agents or generate complexing agents during degradation, and should be considered with regard to the safety function of SFR. Their assessment has been updated, and Appendix A details the selection of chemicals included in this report. The main change is the exclusion of cement additives and tall fatty acids from being considered as potential sources of ISA. Fanger et al. (2001) assumed conservatively that lignin-based cement additives were cellulosic, although lignin and cellulose have very different chemical structures. Similarly, there is no evidence that tall fatty acids can degrade to ISA. In this report, only cellulose and the methoxycellulose additive Methocel, which has been used in the grout around the waste packages in the Silo (5.2 tonnes; Fanger et al. 2001), are included as sources of ISA. Furthermore, picolinate, which was reported in Ringhals wastes (R.10, R.15, R.16) by Fanger et al. (2001), has been removed from this analysis as it was only used during the 1998 reference year, thus has little relevance to the SFR as a whole. In recent years, NTA has been substituted with methylglycine diacetic acid (MGDA) in various detergents, by the producers. MGDA is structurally very similar to NTA, see Figure 3-1, and has therefore been included in the NTA concentration calculations where the usage has been confirmed. Therefore, concentrations have calculated for cellulose and Methocel (generating ISA), citrate, gluconate, EDTA, NTA (including MGDA), oxalate and sodium capryliminodipropionate (NKP).

This section compiles the cellulose and complexing agent content of the different waste package types intended for disposal in 1 and 2BMA, the Silo and 1 and 2BTF vaults. The code system defining the waste types and their characteristics is explained in detail in the Initial State Report (SKB 2014b). The concentrations of each complexing agent in each reference waste package and each compartment of 1BMA, caisson of 2BMA, the entire Silo and entire BTF are then calculated.

The BLA waste packages and vaults are not considered in detail due to their very low radionuclide inventories (~0.2% of the total radionuclide inventory in SFR; SKB 2013), and because radionuclide sorption is not a BLA safety function. However, high ISA concentrations could be of interest in terms of their potential influence on other repository parts. 1BLA will have a high pH over the time period relevant for cellulose degradation (Cronstrand 2014). Given the large amounts of cellulose present in this vault and the more limited amount of concrete compared to the other vaults, α-ISA concentrations are likely to be controlled by precipitation of Caα-ISA$_2$. 2-5BLA wastes are likely to contain both cellulose and a large amount of concrete. However, the mass of cellulose that will be deposited is highly uncertain as the wastes will be generated during the future decommissioning of plants, and steps may be taken to lower the cellulose content through avoidance of cellulosic materials and/or waste treatment of cellulose, such as incineration. Therefore, for 2-5BLA, indicative masses of cellulose have been calculated that correspond to different ISA concentrations in the vaults.
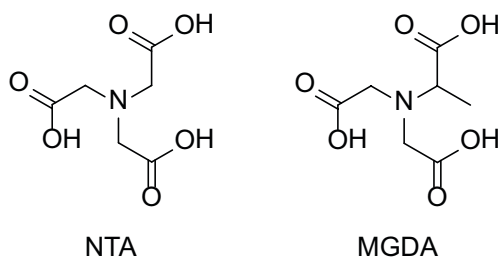
Figure 3-1. *Chemical structures of NTA and MGDA.*

3.1 Inputs of cellulose and complexing agents

The mass of cellulose and complexing agents disposed of in each type of waste package is compiled in this section.

3.1.1 Cellulose

As discussed in Section 2.3, cellulose is an important consideration for the SFR safety case due to its in situ degradation to ISA. Significant quantities of cellulose are present in SFR through the disposal of materials such as contaminated paper, textiles and wood. The estimated maximum masses of cellulose in different waste types of 1 and 2BMA, the Silo and 1BTF (SKB 2013) are reported in Table 3-1, note that only the waste types that contain cellulose are listed. No cellulose is present in 2BTF wastes. Table 3-1 includes four new waste packages, with respect to Fanger et al. (2001): types B.23 and B.23:Dsec in the BMA, and R.24 and S.24 in the Silo. The "Dsec" suffix indicates secondary waste from decommissioning. Also, the cellulose content of the reference waste package types C.01, F.17 and O.01 in the BMA, and O.24 in the Silo, has changed since Fanger et al. (2001). Finally, O.99:1 and some R.23 waste packages are now assigned to 1BTF and contain cellulose.

Appendix B, Table B-1 shows the distribution of waste packages in the 1BMA compartments and Appendix B, Table B-2 shows the mass of cellulose in each 1BMA compartment and the 1 and 2BMA, Silo and 1BTF vaults. The Silo contains 5,200 kg of Methocel cement additive in the construction concrete, which contributes to its cellulose content.

Table 3-1. Mass of cellulose in the relevant waste packages of 1 and 2BMA, the Silo and 1BTF (SKB 2013). When only a sub-group of a waste package type contains cellulose, the suffix "_cell" is applied. "_C" and "_S" denote concrete and steel packaging when both are possible for a given waste type.

Waste package	Type of packaging	Number anticipated at closure that contain cellulose		Waste conditioning	Cellulose (kg package⁻¹)
1 and 2BMA		**1BMA**	**2BMA**		
B.23	Steel with concrete lid	33	0	Concrete	44
B.23:Dsec	Steel with concrete lid	0	122	Concrete	44
C.01_cell	Concrete	61	0	Cement	20.5
C.23	Concrete	63	98	Concrete	30
F.17_cell	Steel	195	0	Bitumen	4.3
F.23_C	Concrete	57	0	Concrete	29
F.23_S	Steel with concrete lid	220	250	Concrete	150
O.01_cell	Concrete	278	0	Cement	20.5
O.23	Concrete	509	100	Concrete	30
R.23_C	Concrete	338	0	Concrete	11
R.23_S	Steel with concrete lid	172	96	Concrete	44
S.21	Steel	488	0	(Concrete between inner and outer containment)	7.9
S.23	Concrete	113	605	Concrete	29
Silo					
C.24	Concrete	350		Concrete	35
O.24	Steel	204		Concrete	5
R.24	Steel	60		Concrete	5
S.11	Steel	106		Cement	3
S.24_C	Concrete	697		Concrete	5
S.24_S	Steel	129		Concrete	5
1BTF					
O.99:1	Steel	40		Cement	21
R.23_C	Concrete	21		Concrete	11

3.1.2 Complexing agents

The complexing agents in SFR mainly arise from the use of detergents. Detergent recipes can change and different detergents have been used at the nuclear sites over time. EDTA use has been banned since 1998, and there are now more stringent limits in place on the disposal of complexing agents in SFR, with large quantities of strong complexing agents banned. The nuclear sites are therefore either modifying their choice of detergent or waste processing techniques. For example, the amount of complexing agents used will be lowered by changing to a floor cleaner based on calcium carbonate. Washing detergents may still contain complexing agents, but these comprise a smaller component of the detergents used at the nuclear sites. Also, at Ringhals (R), all evaporator residues will be electrochemically degraded to break down the complexing agents used. Therefore, the majority of complexing agents that will be disposed in SFR at closure come from pre-2012 activities.

The nuclear power plants and other nuclear facilities have provided improved information on their use of complexing agents for this report. The waste streams have also been critically evaluated to identify the waste packages that receive these complexing agents more accurately. The information provided is as follows:

- Forsmark provided data on the amount of every detergent used from 1987 to the end of 2011, and the complexing agent content of these has been divided equally into each waste package of F.17 produced up to the end of 2011 (Table 3-2).

- Ringhals provided equivalent data for the period 1976–2010, and the complexing agent content of this was divided equally by mass into all packages of R.10, R.15 and R.16 produced up to the end of 2010.

- Barsebäck assessed the gluconate content of 10 packages of a sub group of B.07 type wastes produced between 2003–2010, and a further package produced in 2011. They also calculated the amount of oxalate deposited of, originating from system decontamination, to be 40 kg. This amount was divided into the B.04 packages produced before 2010.

- Oskarshamn assessed the concentration of NTA in their O.07 type wastes, and gave a maximum concentration for the wastes produced over ten years at a rate of 11 waste packages per year. They also calculated the amount of oxalate deposited of, originating from system decontamination, to be 50 kg up to the end of 2010. This amount was divided into the 346 O.02 packages produced between 1990–2010.

- The Central Interim Storage for Spent Fuel (Clab) in Oskarshamn provided data for their 2009 detergent use, which was divided into the number of C.02 waste packages produced in a year.

- The complexing agents used at Studsvik will not be deposited in the vaults considered in this report. S.09 is no longer destined for 1BMA.

The mass of each complexing agent in each waste type is given in Table 3-2 alongside the number of waste packages that contain complexing agents. Since the complexing agents in B.07 and O.07 waste packages have been assessed in two distinct time periods (Fanger et al. 2001) and the 2000s (as described above), Table 3-2 shows the maximum mass of each chemical per package identified in either period.

As reported in Fanger et al. (2001), an estimated total of 10 kg of EDTA has been deposited at SFR, in waste packages produced by 1998. As before, this EDTA is assumed to have been used equally at the four nuclear power plants. The 2.5 kg from each site was then divided equally into the following waste package types produced prior to the end of 1998: B.07, Barsebäck; F.17, Forsmark; O.07, Oskarshamn, and; R.10, R.15 and R.16, Ringhals. The mass of complexing agents in each 1BMA compartment and the 1 and 2BMA, Silo and 1BTF vaults are given in Appendix B, Table B-2.

Table 3-2. Mass of complexing agents per waste package in SFR. Note that O.07 and B.07 show the maximum concentration of each complexing agent identified in either 1998 or the recent assessment. EDTA is only present in waste packages produced up to the end of 1998.

Waste type	Type of packaging	Number of waste packages that contain complexing agents	EDTA	NKP [a]	NTA	Citrate	Oxalate	Sodium-gluconate
1BMA			kg waste package^{-1}					
F.17	Steel	608	$7.1 \cdot 10^{-3}$		$6.9 \cdot 10^{-1}$ [b]	$3.2 \cdot 10^{-1}$	$1.7 \cdot 10^{-2}$	$7.0 \cdot 10^{-2}$
R.10	Concrete	84	$2.9 \cdot 10^{-3}$		$1.1 \cdot 10^{0}$			$1.3 \cdot 10^{-1}$
R.15	Steel with concrete lid	147	$2.9 \cdot 10^{-3}$		$1.1 \cdot 10^{0}$			$1.3 \cdot 10^{-1}$
Silo								
B.04	Steel	349					$1.1 \cdot 10^{-1}$	
C.02	Concrete	416			$6.8 \cdot 10^{-2}$			
O.02	Concrete	346					$1.4 \cdot 10^{-1}$	
R.16	Steel with concrete lid	1,445 [c]	$2.9 \cdot 10^{-3}$		$1.1 \cdot 10^{0}$			$1.3 \cdot 10^{-1}$
1 and 2BTF								
B.07	Concrete	223	$1.3 \cdot 10^{-2}$		$3.5 \cdot 10^{-4}$	$2.5 \cdot 10^{-1}$		$3.1 \cdot 10^{-1}$ [d]
O.07	Concrete	527	$6.3 \cdot 10^{-3}$	$7.7 \cdot 10^{-1}$	$1.6 \cdot 10^{0}$	$4.0 \cdot 10^{-2}$		$1.0 \cdot 10^{0}$

[a] Sodium dicapryliminodipropionate, information from Fanger et al. (2001).

[b] Includes MGDA, which has a very similar structure to NTA.

[c] 664 of these contain EDTA.

[d] Maximum amount of gluconate anticipated within one waste package in 2011; the 10 waste packages produced 2003–2010 contained an estimated 0.028 kg waste package^{-1}, gluconate was not used at Barsebäck prior to 2003.

3.2 Estimates of the void and pore volume, and mass of hydrated cement in each SFR unit considered

In order to calculate the concentration of ISA and other complexing agents in the waste packages and larger units of SFR, it is necessary to estimate the volume of water that will be present in each unit once the repository has re-saturated. Generic pore and void volumes for wastes packaged in each type of packaging have been calculated for the Initial State Report (SKB 2014b). Therefore, the approach used here follows this as far as possible, while retaining a waste type by waste type analysis. Estimates of the amount of hydrated cement in each waste package and unit are also required to account for sorption of ISA and gluconate.

3.2.1 Calculation of the pore and void volumes of the wastes, packaging and repository parts

The different waste materials disposed in SFR vary in porosity, and the waste package types vary in size, conditioning (bitumen, cement, concrete, none), packaging material (concrete or steel) and void volume. The total pore and void volume equates to the volume of water that will be present, post re-saturation of SFR. The void is considered to be the empty space around the waste/conditioned waste while the pore volume reflects the space within the waste/conditioned waste.

The total pore and void volume inside each waste package was calculated using Equation 3-1, while the total pore and void volume of the package, including the packaging, was calculated using Equation 3-2. To differentiate between the concentrations calculated in the waste and the entire waste package, the inclusion of the packaging material is mentioned specifically throughout this report. The data used for the different components of the equations are described below.

$Pore\ and\ void\ volume_{inside\ a\ waste\ package} =$

$PV_{waste\ and\ conditioning} + VV_{waste\ package}$

Equation 3-1

where

PV = pore volume; VV = void volume.

Pore and void volume$_{waste\ package}$ =
$PV_{waste\ and\ conditioning} + VV_{waste\ package} + PV_{packaging}$ Equation 3-2

The Waste Inventory Report (SKB 2013) provides the following relevant information for each waste package:

- Void volume.

- Outer volume of the packaging material.

- Type of packaging material.

- Mass of concrete in the packaging.

- Mass of cement, concrete or bitumen conditioning material.

- Mass of each type of waste component.

The inner volume of each type of waste package is given in the Initial State Report (SKB 2014b).

The Initial State Report (SKB 2014b) also describes the distribution of waste packages between the different SFR vaults and 1BMA compartments at closure (Appendix B, Table B-1).

Pore volume of the packaging material

First, the volume of the packaging material was calculated for each waste type by subtracting the inner volume from the outer volume of the packaging material. This was then multiplied by the porosity of concrete packaging (Table 3-3). For steel containers with concrete lids, the mass of concrete in the lid was converted into a pore volume by ratio with the mass of concrete in the concrete containers. The results are given in Appendix B, Table B-3.

Void volume of the waste in the Silo, 1BMA and 2BMA

The void volume in each waste package was taken directly from the Waste Inventory Report (SKB 2013).

Pore volume of the waste in the Silo, 1BMA and 2BMA

All wastes in the Silo, 1BMA and 2BMA are conditioned prior to disposal. Following the approach in the Initial State Report (SKB 2014b), the volume of conditioned waste in each waste package was calculated by subtracting the void volume in each waste package from the inner volume of the package. The pore volume was then calculated as 15% of the volume of conditioned waste, with the exception of bitumen stabilised ion-exchange resins from Forsmark. Bitumen-conditioned ion-exchange resins from Forsmark were assigned a porosity of zero as they are dried prior to conditioning and water will not penetrate the bitumen significantly. For steel containers with concrete lids, the pore volume of the lid was subtracted from the pore volume of the waste, as these lids are not differentiated from the waste in the Initial State Report (SKB 2014b). The pore volume of the waste was calculated for each type of waste package here individually, while in the Initial State Report it was calculated for generic concrete moulds, steel moulds and steel drums. The results are given in Appendix B, Table B-3

Pore volume of the waste in 1 and 2BTF

1 and 2BTF contain a range of conditioned and unconditioned waste materials. Some of the conditioned wastes (O.01, R.01, R.10 and R.23_C) are of a type primarily disposed of in BMA. However, a limited number of these packages are used to create supporting walls around the S.13 drums in 1BTF. The pore and void volumes of these were calculated as above. For the other wastes, the pore volumes in the conditioning cement, concrete waste and ion-exchange resins were calculated separately from the mass given in the Waste Inventory Report (SKB 2013), and the densities and porosities given in Table 3-3, and then summed.

Table 3-3. Characteristics of the waste materials, waste conditioning, packaging and construction concrete in SFR.

Parameter	Component	Value
Mass of hydrated cement in concrete (kg kg^{-1})	Concrete conditioning for scrap metal and refuse	0.38
	Cement conditioning for other waste types	1
Mass of hydrated cement in concrete (kg m^{-3})	Construction concrete	515
	Concrete packaging	515
	Silo/BMA grout	691
	BTF grout	528
Porosity (%)	Construction concrete	15
	Concrete packaging	15
	Steel packaging	0
	Silo conditioned waste	15
	BMA conditioned waste	15
	Forsmark bitumen-conditioned waste	0
	BTF concrete/cement conditioning	20
	BTF ion-exchange resins	40
	Other BTF wastes	0
Bulk density (kg m^{-3}; applied to BTF)	Cement conditioning	2,000
	Concrete conditioning	2,000
	Concrete waste	2,300
	Ion-exchange resins	1,000

Here, consistency with the Initial State Report (SKB 2014b) was maintained by using the same values for the pore volume for ion-exchange resins and void volume for the reactor tank lid (R.99:1). However, the handling of S.13 (concrete-conditioned ashes) introduced a small discrepancy. The results are given in Appendix B, Table B-3

Pore and void volume of larger units of SFR

The waste distribution (SKB 2013, 2014b) was used to calculate the total pore and void volume in the waste contained in each larger unit of SFR (i.e. BMA compartment/caisson or vault), and the values were compared with those given in the Initial State Report (SKB 2014b). There was close agreement between the values for the Silo, 1BMA and 2BTF (<0.4% variation). However, there was slightly higher variation between the values for 2BMA caissons (1.2%), due to the generalised approach in the Initial State Report (SKB 20114b), and for 1BTF (4%), due to the different handling of the S.13 waste type. For 2BMA caissons, the numerical difference between the waste values is balanced by a nearly equal and opposite difference in the pore volumes calculated for the grout.

As small differences do not affect the concentrations calculated here (reported to 2 significant figures), the volumes and pore volumes of each structural unit of SFR were taken from the Initial State Report for consistency. However, for 1BTF, the additional pore volume in the waste was added to the pore and void volumes given in the Initial State Report for the vault. The units of SFR considered were the rock vaults, the 1BMA compartments, 2BMA caissons and the Silo construction, all of which included the concrete construction material, and the 1BTF waste zone, defined by the grouted volume including the concrete floor and lid. The values used are given in Appendix B, Table B-4.

3.2.2 Calculation of the hydrated cement content of the wastes, packaging and repository parts

The mass of hydrated cement (HC) inside each waste package and in each waste package, including the packaging material were calculated using Equation 3-3 and Equation 3-4, respectively.

$$HC_{inside\ a\ waste\ package} = HC_{waste\ materials} + HC_{conditioning} \qquad \text{Equation 3-3}$$

$$HC_{waste\ package} = HC_{waste\ materials} + HC_{conditioning} + HC_{packaging} \qquad \text{Equation 3-4}$$

The mass of concrete waste and cement and concrete conditioning in each waste package type was extracted from the Waste Inventory Report (SKB 2013). The mass of hydrated cement in each of these was then calculated using the values given in Table 3-3 (mass per kg). The mass of hydrated cement in the packaging was calculated from the volume of concrete in the packaging (see above) and the mass of hydrated cement per m^3 (Table 3-3) and the results are given in Appendix B, Table B-3.

For SFR vaults, the mass of hydrated cement was calculated using Equation 3-5, and for smaller units within a vault, i.e. 1BMA compartments, 2BMA caissons, the Silo construction and the 1BTF waste zone, the relevant components of this were summed.

$$HC_{vault} = HC_{waste\ packages} + HC_{structural\ concrete} + HC_{backfill\ concrete} + HC_{shotcrete} \qquad \text{Equation 3-5}$$

The volume of hydrated cement in the waste packages was calculated using the information for the different waste packages types (Appendix B, Table B-3) and the distribution of the waste packages into the different rock vaults (SKB 2013) and 1BMA compartments (SKB 2014b, shown in Appendix B, Table B-1). The volumes of structural concrete, grout and shotcrete in each unit were taken from the Initial State Report (SKB 20114b) and converted into masses of hydrated cement using the relevant conversion value (mass of hydrated cement per m^3), given in Table 3-3. It was assumed that the 2BMA caissons would be filled with waste in turn, and the current waste assigned to 2BMA would fill 8.4 caissons (SKB 2014b). Therefore, the hydrated cement in the waste was divided by 8.4 to obtain the mass per caisson. The results of the calculations are given in Appendix B, Table B-4.

3.3   Concentration calculations

In this section, the concentrations of potentially important complexing agents are given within the porewater of each waste type and defined repository parts. The calculations assume 100% release of the complexing agents from the waste matrix into the porewater. However, the concentrations of gluconate were also calculated following sorption to the available hydrated cement, using Equation 2-3. In the case of ISA, the porewater concentration was calculated from the mass of cellulose present and the extent of cellulose degradation as a function of time (Equation 2-1). The porewater ISA concentrations were also calculated following sorption of ISA to available hydrated cement (Equation 2-3).

3.3.1   Concentrations of ISA

Using the cellulose degradation constants derived for Tela tissues, the model of Glaus and Van Loon (2008) predicts that 4, 11, 38, 60 and 99% of the cellulose in highly alkaline parts of SFR will have degraded after 10, 100, 500, 1,000 and 5,000 years, respectively (see Section 2.2.1). Since ISA comprises ~80% of cellulose degradation products (Bradbury and Van Loon 1997, Van Loon and Glaus 1997, 1998, Pavasars et al. 2003, Glaus and Van Loon 2008), the mass of ISA produced was calculated as 3.2, 9.0, 30, 48 and 79% of the cellulose present inside each waste package. The assumption that ISA does not migrate out from each waste package over time is conservative, especially at the longer time intervals considered. For waste type F.17, the approach also assumes that alkaline water enters the package, which would only occur after degradation or damage of the package. Degradation of ISA has not been accounted for, due to the lack of evidence that degradation occurs under alkaline, anaerobic conditions (Section 2.3.1).

The sorption calculations applied the non linear two site sorption isotherm described in Section 2.3.1 (Equation 2-3). All of the ISA was included in the sorption calculations, as α- and β-ISA have comparable sorption isotherms (Van Loon and Glaus 1998).

There is evidence that Eu(III) forms more stable complexes with α-ISA than β-ISA (Van Loon and Glaus 1998), which suggests that the α-ISA concentration should be reported. However, the total ISA concentrations are reported here for the following reasons:

- ISA is not always separated into its diastereoisomers for radionuclide sorption experiments

- α-ISA is expected to precipitate at concentrations above $2 \cdot 10^{-2}$ M under portlandite-controlled conditions and, when this happens, the ratio of α-ISA: β-ISA will vary between the precipitated, solution and sorbed phases. There has been no experimental investigation of this.

- Sorption of ISA to cement means that the impact of ISA on radionuclide sorption is highly sensitive to the experimental design

- The data suggesting that β-ISA is a weaker complexing agent than α-ISA is relatively limited, and the stability constant for the Eu β-ISA complex in Van Loon and Glaus (1998) was still reasonably high

However, where appropriate, the solubility limit for α-ISA is referred to in the results tables to highlight that further increases above this concentration are not likely to equate to a linear increase in complexing power. Note that since the tables show the total concentration of ISA, and α-ISA comprises approximately half of this, the solubility limit for α-ISA is considered to have been reached when the total ISA concentration is twice this limit.

The concentrations of ISA after 5,000 years of cellulose degradation, in the pore and void volume inside the waste packages and in the complete waste packages, including the packaging, are given in Table 3-4. Table 3-4 also shows the concentrations following sorption of ISA to the available hydrated cement.

Table 3-4. Concentrations of ISA calculated after 5,000 years of cellulose degradation inside the relevant BMA, Silo and BTF waste packages and in the packages including the packaging material. The ISA concentrations were calculated with and without consideration of sorption to available hydrated cement. When the calculated ISA concentration was more than twice the expected solubility limit for α-ISA during the portlandite stage of cement degradation ($2 \cdot 10^{-2}$ M), i.e. $4 \cdot 10^{-2}$ M, the solubility limit is given followed by the calculated concentration in brackets. Steel packaging has no influence on the concentrations calculated.

| | ISA Concentration (M) | | | |
| | Inside the was te package | | Including the packaging material | |
	No sorption	Sorption	No sorption	Sorption
1 and 2BMA				
B.23	$2 \cdot 10^{-2}$ ($3.3 \cdot 10^{-1}$)	$2 \cdot 10^{-2}$ ($1.5 \cdot 10^{-1}$)	$2 \cdot 10^{-2}$ ($3.1 \cdot 10^{-1}$)	$2 \cdot 10^{-2}$ ($1.1 \cdot 10^{-1}$)
B.23:Dsec	$2 \cdot 10^{-2}$ ($3.3 \cdot 10^{-1}$)	$2 \cdot 10^{-2}$ ($1.5 \cdot 10^{-1}$)	$2 \cdot 10^{-2}$ ($3.1 \cdot 10^{-1}$)	$2 \cdot 10^{-2}$ ($1.1 \cdot 10^{-1}$)
C.01_cell	$2 \cdot 10^{-2}$ ($2.1 \cdot 10^{-1}$)	$7.6 \cdot 10^{-4}$	$2 \cdot 10^{-2}$ ($1.7 \cdot 10^{-1}$)	$4.9 \cdot 10^{-4}$
C.23	$2 \cdot 10^{-2}$ ($3.6 \cdot 10^{-1}$)	$2 \cdot 10^{-2}$ ($2.3 \cdot 10^{-1}$)	$2 \cdot 10^{-2}$ ($2.8 \cdot 10^{-1}$)	$2 \cdot 10^{-2}$ ($6.3 \cdot 10^{-2}$)
F.17_cell	$2 \cdot 10^{-2}$ ($1.1 \cdot 10^{-1}$)	$2 \cdot 10^{-2}$ ($1.1 \cdot 10^{-1}$)	$2 \cdot 10^{-2}$ ($1.1 \cdot 10^{-1}$)	$2 \cdot 10^{-2}$ ($1.1 \cdot 10^{-1}$)
F.23_C	$2 \cdot 10^{-2}$ ($3.5 \cdot 10^{-1}$)	$2 \cdot 10^{-2}$ ($2.2 \cdot 10^{-1}$)	$2 \cdot 10^{-2}$ ($2.7 \cdot 10^{-1}$)	$2 \cdot 10^{-2}$ ($5.8 \cdot 10^{-2}$)
F.23_S	$2 \cdot 10^{-2}$ ($1.1 \cdot 10^{0}$)	$2 \cdot 10^{-2}$ ($8.9 \cdot 10^{-1}$)	$2 \cdot 10^{-2}$ ($1.1 \cdot 10^{0}$)	$2 \cdot 10^{-2}$ ($8.1 \cdot 10^{-1}$)
O.01_cell	$2 \cdot 10^{-2}$ ($2.1 \cdot 10^{-1}$)	$7.6 \cdot 10^{-4}$	$2 \cdot 10^{-2}$ ($1.7 \cdot 10^{-1}$)	$4.9 \cdot 10^{-4}$
O.23	$2 \cdot 10^{-2}$ ($3.6 \cdot 10^{-1}$)	$2 \cdot 10^{-2}$ ($2.3 \cdot 10^{-1}$)	$2 \cdot 10^{-2}$ ($2.8 \cdot 10^{-1}$)	$2 \cdot 10^{-2}$ ($6.3 \cdot 10^{-2}$)
R.23_C	$2 \cdot 10^{-2}$ ($1.3 \cdot 10^{-1}$)	$2 \cdot 10^{-2}$ ($4.1 \cdot 10^{-2}$)	$2 \cdot 10^{-2}$ ($1.0 \cdot 10^{-1}$)	$1.9 \cdot 10^{-3}$
R.23_S	$2 \cdot 10^{-2}$ ($3.3 \cdot 10^{-1}$)	$2 \cdot 10^{-2}$ ($1.5 \cdot 10^{-1}$)	$2 \cdot 10^{-2}$ ($3.1 \cdot 10^{-1}$)	$2 \cdot 10^{-2}$ ($1.1 \cdot 10^{-1}$)
S.21	$2 \cdot 10^{-2}$ ($1.3 \cdot 10^{0}$)	$2 \cdot 10^{-2}$ ($9.6 \cdot 10^{-1}$)	$2 \cdot 10^{-2}$ ($1.3 \cdot 10^{0}$)	$2 \cdot 10^{-2}$ ($9.6 \cdot 10^{-1}$)
S.23	$2 \cdot 10^{-2}$ ($6.1 \cdot 10^{-1}$)	$2 \cdot 10^{-2}$ ($3.7 \cdot 10^{-1}$)	$2 \cdot 10^{-2}$ ($4.0 \cdot 10^{-1}$)	$2 \cdot 10^{-2}$ ($7.1 \cdot 10^{-2}$)
Silo				
C.24	$2 \cdot 10^{-2}$ ($4.2 \; 10^{-1}$)	$2 \cdot 10^{-2}$ ($1.9 \; 10^{-1}$)	$2 \cdot 10^{-2}$ ($3.3 \; 10^{-1}$)	$2 \cdot 10^{-2}$ ($5.7 \cdot 10^{-2}$)
O.24	$2 \cdot 10^{-2}$ ($4.3 \cdot 10^{-2}$)	$3.6 \cdot 10^{-4}$	$2 \cdot 10^{-2}$ ($4.3 \cdot 10^{-2}$)	$3.6 \cdot 10^{-4}$
R.24	$3.5 \cdot 10^{-2}$	$3.6 \cdot 10^{-4}$	$3.5 \cdot 10^{-2}$	$3.6 \cdot 10^{-4}$
S.11	$4.0 \cdot 10^{-2}$	$1.3 \cdot 10^{-4}$	$4.0 \cdot 10^{-2}$	$1.3 \cdot 10^{-4}$
S.24_C	$2 \cdot 10^{-2}$ ($6.1 \cdot 10^{-2}$)	$1.8 \cdot 10^{-3}$	$2 \cdot 10^{-2}$ ($4.7 \cdot 10^{-2}$)	$2.9 \cdot 10^{-4}$
S.24_S	$2 \cdot 10^{-2}$ ($4.3 \cdot 10^{-2}$)	$3.6 \cdot 10^{-4}$	$2 \cdot 10^{-2}$ ($4.3 \cdot 10^{-2}$)	$3.6 \cdot 10^{-4}$
1BTF				
O.99:1	$2 \cdot 10^{-2}$ ($1.2 \; 10^{-1}$)	$2.8 \cdot 10^{-4}$	$2 \cdot 10^{-2}$ ($1.2 \; 10^{-1}$)	$2.8 \cdot 10^{-4}$
R.23_C	$2 \cdot 10^{-2}$ ($1.3 \; 10^{-1}$)	$2 \cdot 10^{-2}$ ($4.1 \cdot 10^{-2}$)	$2 \cdot 10^{-2}$ ($1.0 \; 10^{-1}$)	$1.9 \cdot 10^{-3}$

The previous assessment (Fanger et al. 2001) considered that the most likely extent of cellulose degradation was 1.8%. Therefore, the ISA concentrations reported here are significantly higher than the equivalent values in Fanger et al. (2001). Sorption of ISA to hydrated cement reduces the ISA concentration effectively in some of the BMA and Silo waste packages. However, in the majority of the relevant waste packages, the mass of ISA predicted to form exceeds the amount that can be removed effectively by the available hydrated cement present. Therefore, sorption only reduces the solution phase concentrations to a relatively small degree.

The ISA concentrations in the BMA waste packages at the five time periods considered, following sorption to the available hydrated cement, are shown in Figure 3-2, and Appendix C, Table C-1 and Table C-2. The solubility limit for α-ISA expected in a cementitious environment (0.02 M), due to the precipitation of Caα-ISA$_2$, is shown by a dotted line in Figure 3-2, and it is clear that the ISA concentrations inside the majority of waste packages will reach this within 1,000 years. The inclusion of concrete packaging material (Figure 3-2 bottom) lowers the concentrations calculated to varying extents.
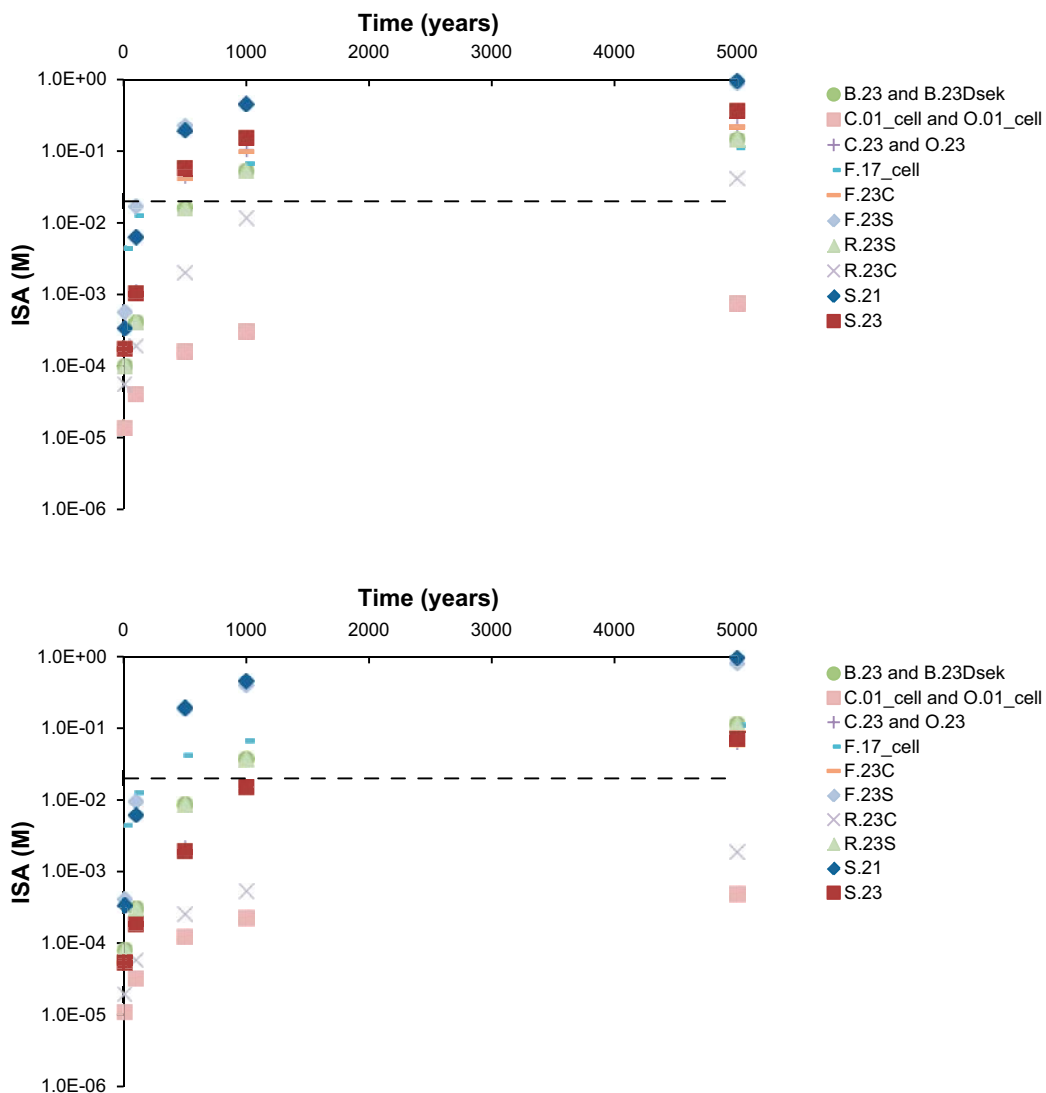

Figure 3-2. *Evolution of the ISA concentrations in BMA waste packages: inside the waste package (top), and including the packaging material (bottom). Sorption of ISA to the hydrated cement in each type of waste package is taken into account. The dashed line shows the solubility limit for α-ISA expected under portlandite-controlled cementitious conditions.*

Table 3-5. Concentrations of ISA calculated in the 1BMA compartments, construction and vault, the 2BMA caissons, the Silo construction and vault, and the 1BTF waste zone and vault, after 5,000 years of cellulose degradation, based on the predicted waste distribution at closure. The ISA concentrations were calculated with and without consideration of sorption to available hydrated cement. When the calculated ISA concentration was more than twice the expected solubility limit for α-ISA during the portlandite stage of cement degradation ($2 \cdot 10^{-2}$ M), i.e. $4 \cdot 10^{-2}$ M, the solubility limit is given, followed by the calculated concentration in brackets.

	ISA Concentration (M)	
	No sorption	Sorption
1BMA compartment		
1	0	0
2	0	0
3	$7.8 \cdot 10^{-3}$	$3.1 \cdot 10^{-5}$
4	$2 \cdot 10^{-2}$ ($9.7 \cdot 10^{-2}$)	$2.7 \cdot 10^{-4}$
5	$4.1 \cdot 10^{-4}$	$1.5 \cdot 10^{-6}$
6	$2.7 \cdot 10^{-3}$	$8.0 \cdot 10^{-6}$
7	$2 \cdot 10^{-2}$ ($6.0 \cdot 10^{-2}$)	$1.5 \cdot 10^{-4}$
8	$2 \cdot 10^{-2}$ ($2.6 \cdot 10^{-1}$)	$1.2 \cdot 10^{-2}$
9	$2 \cdot 10^{-2}$ ($1.2 \cdot 10^{-1}$)	$4.6 \cdot 10^{-4}$
10	$2 \cdot 10^{-2}$ ($1.4 \cdot 10^{-1}$)	$9.2 \cdot 10^{-4}$
11	$2 \cdot 10^{-2}$ ($1.1 \cdot 10^{-1}$)	$5.2 \cdot 10^{-4}$
12	$2 \cdot 10^{-2}$ ($1.1 \cdot 10^{-1}$)	$5.2 \cdot 10^{-4}$
13	$2 \cdot 10^{-2}$ ($1.1 \cdot 10^{-1}$)	$5.3 \cdot 10^{-4}$
14	$2 \cdot 10^{-2}$ ($1.1 \cdot 10^{-1}$)	$5.1 \cdot 10^{-4}$
15	$2 \cdot 10^{-2}$ ($1.1 \cdot 10^{-1}$)	$5.1 \cdot 10^{-4}$
Total 1BMA construction	$2 \cdot 10^{-2}$ ($7.8 \cdot 10^{-2}$)	$2.9 \cdot 10^{-4}$
1BMA vault incl. macadam and shotcrete	$2.3 \cdot 10^{-2}$	$2.7 \cdot 10^{-4}$
2BMA		
2BMA per caisson (waste deposited in 8.4 caissons)	$2 \cdot 10^{-2}$ ($6.0 \cdot 10^{-2}$)	$2.6 \cdot 10^{-4}$
Silo		
Within the outer walls of the Silo construction	$1.6 \cdot 10^{-2}$	$4.5 \cdot 10^{-5}$
Silo construction	$1.4 \cdot 10^{-2}$	$3.8 \cdot 10^{-5}$
Entire vault	$8.1 \cdot 10^{-3}$	$3.8 \cdot 10^{-5}$
1BTF		
Waste zone	$1.5 \cdot 10^{-3}$	$4.7 \cdot 10^{-6}$
Entire vault	$7.3 \cdot 10^{-4}$	$4.5 \cdot 10^{-6}$

Table 3-5 shows the concentrations of ISA calculated for larger units within the SFR vaults, based on the waste distribution at closure given in the Initial State Report (SKB 2014b). In each case, ISA concentrations have been predicted based on an 80% yield from cellulose degradation, with 99% cellulose degradation after 5,000 years. The assumption that ISA does not migrate out from each vault over time appears conservative, especially at the longer time intervals considered. However, a modelling study suggests that 90% of the ISA produced in 1BMA will be retained over a 20,000 year period, due to the sorption of ISA (Von Schenck and Källström 2013). It should be noted that not all waste type descriptions are currently approved for disposal, including B.23, B.23:D, C.24, O.24, R.24, S.21, S.23 and S.24. The ISA concentrations remain below the expected solubility limit for α-ISA in all units considered when sorption is taken into account. However, the concentration in1BMA compartment 8 approaches the solubility limit. The temporal evolution of the ISA concentrations are shown in Figure 3-3 and the data are provided in Appendix C, Table C-3.

3.3.2 Concentrations of gluconate

Gluconate undergoes sorption to hydrated cement (see Section 2.3.1), following the non linear two site Langmuir isotherm (Equation 2-3) and the sorption constants reported in Glaus et al. (2006; also see Section 2.3.1). The concentrations of gluconate inside the BMA, Silo and BTF waste packages (not including the packaging), with and without sorption to the waste conditioning, are presented in Table 3-6.
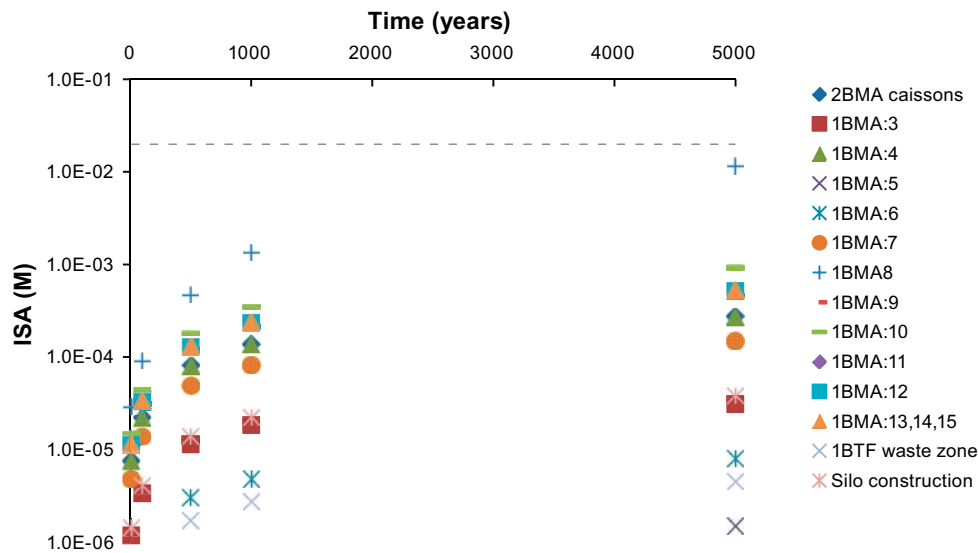
Figure 3-3. *The evolution of the ISA concentration in the 1BMA compartments, 2BMA caissons, 1BTF waste zone and the Silo construction accounting for sorption to hydrated cement. The dashed line shows the solubility limit for α-ISA expected under portlandite-controlled cementitious conditions.*

Table 3-6. Concentrations of gluconate (M) inside the relevant 1BMA, Silo and 1 and 2BTF waste packages and in the packages including the packaging material. The concentrations were calculated with and without consideration of sorption to hydrated cement.

| | Gluconate Concentration (M) | | | |
| | Inside the waste package | | Including the packaging material | |
	No sorption	Sorption	No sorption	Sorption
1BMA				
F.17	$1.9 \cdot 10^{-3}$	$1.9 \cdot 10^{-3}$	$1.9 \cdot 10^{-3}$	$1.9 \cdot 10^{-3}$
R.10	$1.4 \cdot 10^{-3}$	$6.8 \cdot 10^{-9}$	$1.1 \cdot 10^{-3}$	$5.1 \cdot 10^{-9}$
R.15	$2.0 \cdot 10^{-3}$	$4.0 \cdot 10^{-9}$	$1.8 \cdot 10^{-3}$	$3.5 \cdot 10^{-9}$
Silo				
R.16	$2.0 \cdot 10^{-3}$	$1.8 \cdot 10^{-8}$	$1.8 \cdot 10^{-3}$	$1.1 \cdot 10^{-8}$
1 and 2BTF				
B.07	$5.3 \cdot 10^{-4}$ *	$5.3 \cdot 10^{-4}$ *	$4.3 \cdot 10^{-4}$*	$8.9 \cdot 10^{-9}$ *
O.07	$1.5 \cdot 10^{-3}$	$1.5 \cdot 10^{-3}$	$1.3 \cdot 10^{-3}$	$3.0 \cdot 10^{-8}$

* Shows the maximum gluconate concentration anticipated inside one waste package from 2011.

The maximum gluconate concentration in 1 package of a sub-class of the B.07 waste type, B.07:1, is shown in Table 3-6. This sub-class is the only part of B.07 waste to contain gluconate and comprises 11 or 12 packages in total. The re-evaluation of the mass of each complexing agent in the different wastes has resulted in an increased mass of gluconate assigned to O.07. However, the concentration is lower than in Fanger at al. (2001) due to a correction of the pore and void volume of the waste package type (Appendix B, Table B-3).

Table 3-6 shows that inside every cement-conditioned waste package, sorption reduces the gluconate concentrations effectively. The cement-conditioned waste types that contain gluconate do not contain cellulose, which avoids the need to assess whether gluconate and ISA compete for surface binding sites. If the concentrations of gluconate in O.07 and B.07 are calculated for the whole waste package, including the pore volume and hydrated cement of the concrete packaging, the concentrations remaining in solution decrease to 10^{-9}–10^{-8} M (Table 3-6).

The bitumen-conditioned F.17 wastes destined for 1BMA are packaged in steel. However, calculations of the gluconate concentrations within the different 1BMA compartments show that dilution and sorption to the hydrated cement lowers the concentration to $\leq 10^{-9}$ M in every case (Table 3-7).

Table 3-7. Concentrations of gluconate inside the relevant 1BMA compartments, the Silo and 1 and 2BTF. The concentrations were calculated with and without consideration of sorption to hydrated cement.

	Gluconate Concentration (M)	
	No sorption	Sorption
1BMA compartment		
1	0	0
2	0	0
3	$1.3 \cdot 10^{-4}$	$1.1 \cdot 10^{-9}$
4	$2.2 \cdot 10^{-4}$	$8.9 \cdot 10^{-10}$
5	$2.4 \cdot 10^{-5}$	$1.9 \cdot 10^{-10}$
6	$2.8 \cdot 10^{-4}$	$1.7 \cdot 10^{-9}$
7	0	0
8	$5.9 \cdot 10^{-5}$	$3.4 \cdot 10^{-10}$
9	$8.1 \cdot 10^{-5}$	$3.8 \cdot 10^{-10}$
10	$4.5 \cdot 10^{-5}$	$2.4 \cdot 10^{-10}$
11	$7.4 \cdot 10^{-5}$	$4.1 \cdot 10^{-10}$
12	$5.6 \cdot 10^{-5}$	$3.1 \cdot 10^{-10}$
13	$5.6 \cdot 10^{-5}$	$3.1 \cdot 10^{-10}$
14	$3.2 \cdot 10^{-5}$	$1.7 \cdot 10^{-10}$
15	$3.2 \cdot 10^{-5}$	$1.7 \cdot 10^{-10}$
Silo		
Silo construction	$1.2 \cdot 10^{-4}$	$6.3 \cdot 10^{-10}$
Entire Silo	$6.7 \cdot 10^{-5}$	$6.3 \cdot 10^{-10}$
1 and 2BTF		
Entire 1 and 2BTF	$1.4 \cdot 10^{-4}$	$2.3 \cdot 10^{-9}$

3.3.3 Concentrations of other complexing agents

The aqueous concentrations of all other complexing agents were calculated using the assumption that they remain in solution, with no sorption to hydrated cement. This approach is cautious, but necessary due to the lack of sorption isotherm data or relevant degradation studies in the literature. Table 3-8 shows that NTA, citrate and oxalate are present at the highest concentrations inside the waste packages, but the oxalate concentration will be controlled by the formation of sparingly soluble calcium oxalate. The concentrations in the waste packages, including the waste packaging material, are given in Appendix C, Table C-4.

The concentrations of EDTA, NKP, NTA, citrate and oxalate were calculated within each compartment of 1BMA, the entire Silo and entire BTF (Table 3-9). Since complexing agents will not be present in the wastes produced at the nuclear power plants after 2012, not all packages of a given waste package type will contain complexing agents. This is readily accounted for in the vaults, and therefore 1 and 2BTF have been considered as one unit. For 1BMA, the waste packages that contain complexing agents have been distributed into the compartments as shown in Appendix B, Table B-5, for the purposes of this report. This takes disposals to date into account and then distributes the remaining packages into appropriate compartments relatively evenly. For the BTF, the different sub-categories of B.07 and O.07 wastes (see Section 3.1.2) were accounted for separately, so that the concentrations were as realistic as possible. However, it should be noted that the mass of NKP in each O.07 waste package from Fanger et al. (2001) was applied to all O.07 waste packages that have received complexing agents, and this introduces uncertainty for the NKP concentration in 1 and 2BTF.

The concentrations shown in Table 3-9 are very variable, and NTA is present at the highest concentrations of these complexing agents, between $1.0 \cdot 10^{-4}$–$3.2 \cdot 10^{-3}$ M.

Table 3-8. Concentrations of other complexing agents inside the different waste packages of 1BMA, the Silo and 1 and 2BTF. When the calculated oxalate concentration is higher than the solubility limit expected under repository conditions, $1\cdot10^{-5}$ M, this maximum is given followed by the calculated concentration in brackets.

| | Complexing agent concentration (M) | | | | |
	EDTA	NKP	NTA	Citrate	Oxalate
1BMA					
F.17	$1.4\cdot10^{-4}$		$2.1\cdot10^{-2}$	$9.8\cdot10^{-3}$	$1\cdot10^{-5}$ ($1.1\cdot10^{-3}$)
R.10	$2.3\cdot10^{-5}$		$1.4\cdot10^{-2}$		
R.15	$3.3\cdot10^{-5}$		$2.0\cdot10^{-2}$		
Silo					
B.04					$1\cdot10^{-5}$ ($2.3\cdot10^{-2}$)
C.02			$8.3\cdot10^{-4}$		
O.02					$1\cdot10^{-5}$ ($3.7\cdot10^{-3}$)
R.16	$3.3\cdot10^{-5}$		$1.9\cdot10^{-2}$		
1 and 2BTF					
B.07*	$1.6\cdot10^{-5}$		$6.7\cdot10^{-7}$	$4.8\cdot10^{-4}$	
O.07*	$7.1\cdot10^{-6}$	$8.5\cdot10^{-4}$	$2.8\cdot10^{-3}$	$6.9\cdot10^{-5}$	

* Note that O.07 and B.07 show the maximum concentration of each complexing agent from the mass identified in either 1998 or the recent assessment.

Table 3-9. Concentrations of other complexing agents in each relevant 1BMA compartment and in the Silo and BTF. When the calculated oxalate concentration is higher than the solubility limit expected under repository conditions, $1\cdot10^{-5}$ M, this maximum is given followed by the calculated concentration in brackets.

| | Complexing agent concentration (M) | | | | |
	EDTA	NKP	NTA	Citrate	Oxalate
1BMA compartment					
1					
2					
3	$1.0\cdot10^{-5}$		$1.5\cdot10^{-3}$	$6.9\cdot10^{-4}$	$1\cdot10^{-5}$ ($7.8\cdot10^{-5}$)
4	$3.6\cdot10^{-6}$		$2.1\cdot10^{-3}$		
5	$1.9\cdot10^{-6}$		$2.8\cdot10^{-4}$	$1.3\cdot10^{-4}$	$1\cdot10^{-5}$ ($1.4\cdot10^{-5}$)
6	$2.1\cdot10^{-5}$		$3.2\cdot10^{-3}$	$1.5\cdot10^{-3}$	$1\cdot10^{-5}$ ($1.7\cdot10^{-4}$)
7					
8	$9.4\cdot10^{-7}$		$5.7\cdot10^{-4}$		
9	$1.3\cdot10^{-6}$		$7.9\cdot10^{-4}$		
10	$3.4\cdot10^{-6}$		$5.0\cdot10^{-4}$	$2.3\cdot10^{-4}$	$1\cdot10^{-5}$ ($2.6\cdot10^{-5}$)
11	$5.0\cdot10^{-6}$		$8.2\cdot10^{-4}$	$3.3\cdot10^{-4}$	$1\cdot10^{-5}$ ($3.7\cdot10^{-5}$)
12	$3.6\cdot10^{-6}$		$6.1\cdot10^{-4}$	$2.3\cdot10^{-4}$	$1\cdot10^{-5}$ ($2.7\cdot10^{-5}$)
13	$3.6\cdot10^{-6}$		$6.1\cdot10^{-4}$	$2.4\cdot10^{-4}$	$1\cdot10^{-5}$ ($2.7\cdot10^{-5}$)
14	$5.2\cdot10^{-7}$		$3.1\cdot10^{-4}$		
15	$5.2\cdot10^{-7}$		$3.1\cdot10^{-4}$		
Total 1BMA construction	$3.8\cdot10^{-6}$		$7.9\cdot10^{-4}$	$2.3\cdot10^{-4}$	$1\cdot10^{-5}$ ($2.6\cdot10^{-5}$)
1BMA vault incl. macadam and shotcrete	$1.1\cdot10^{-6}$		$2.4\cdot10^{-4}$	$6.8\cdot10^{-5}$	$7.7\cdot10^{-6}$
Silo					
Within the outer walls of the Silo construction	$1.0\cdot10^{-6}$		$1.3\cdot10^{-3}$		$1\cdot10^{-5}$ ($1.5\cdot10^{-4}$)
Silo construction	$9.1\cdot10^{-7}$		$1.2\cdot10^{-3}$		$1\cdot10^{-5}$ ($1.4\cdot10^{-4}$)
Entire vault	$5.2\cdot10^{-7}$		$6.6\cdot10^{-4}$		$1\cdot10^{-5}$ ($8.0\cdot10^{-5}$)
1 and 2BTF					
Entire vaults	$1.3\cdot10^{-6}$	$7.7\cdot10^{-5}$	$1.0\cdot10^{-4}$	$2.7\cdot10^{-5}$	

3.4   Cellulose in 2-5 BLA

2-5BLA will contain large amounts of concrete waste, which may result in sufficiently alkaline conditions for significant cellulose degradation and generation of ISA. It is currently difficult to predict the cellulose content of the secondary waste with accuracy, and it is likely that steps will be taken to use alternative materials or treat cellulosic waste prior to disposal. Here, the pore and void volume of 2-5 BLA has been taken from the Initial State Report (SKB 2014b). The mass of hydrated cement has been calculated from the volumes of cementitious materials given in the Initial State Report (SKB 2014b) and the mass of hydrated cement in each of these materials, given in Table 3-3. The hydrated cement in the wastes has been calculated from the mass of concrete waste and/or conditioning in each waste type and the prediction of the number of each waste type to be deposited in 2-5BLA at closure (SKB 2013). The values for the total mass of hydrated cement and the total pore and void volume in 2-5 BLA allow calculation of the mass of cellulose in 2-5BLA that corresponds to specific ISA concentrations after 5,000 years. This applies the very pessimistic assumption for these vaults that the system will be "tight" over long periods of time. The mass of cellulose has been calculated for three ISA concentrations, with sorption to the available hydrated cement taken into account (Table 3-10).

Table 3-10. Mass of cellulose in 2-5BLA that will generate specified ISA concentrations. Sorption to the available hydrated cement has been taken into account.

ISA concentration (M)	Hydrated cement (kg)	Pore and void volume (m^3)	Mass of cellulose (kg)
$1.00 \cdot 10^{-2}$	$3.36 \cdot 10^6$	$5.00 \cdot 10^4$	$2.00 \cdot 10^5$
$1.00 \cdot 10^{-3}$	$3.36 \cdot 10^6$	$5.00 \cdot 10^4$	$6.15 \cdot 10^4$
$1.00 \cdot 10^{-4}$	$3.36 \cdot 10^6$	$5.00 \cdot 10^4$	$1.26 \cdot 10^4$

4 Summary

4.1 ISA

The concentrations of ISA calculated in this report exceed those of Fanger et al. (2001) significantly, due to the higher ISA yields applied in the cellulose degradation calculations. Within the majority of cellulose-containing 1 and 2BMA waste package types, the ISA concentrations calculated exceed the expected solubility limit for α-ISA in SFR after 1,000 years, even after sorption to the available hydrated cement has been taken into account. Dilution into the waste packaging material and further sorption reduces the concentrations to an extent and, when the different compartments/caissons of BMA, the Silo and 1BTF are considered, the dissolved ISA concentrations are reduced to a maximum of $1.2 \cdot 10^{-2}$ M (1BMA compartment 8). The ISA data are upper limits, since the maximum mass of cellulose in each waste package was used in the calculations. It should also be noted that the extrapolation of experimental cellulose degradation data from 12 to 5,000 years, and the assumption of ISA stability over this time, contribute further to the cautious nature of these data. Finally, it should be noted that the α-ISA concentration comprises half of the ISA concentration in each compartment/caisson of BMA, the Silo and 1BTF, since no precipitation occurs in these repository parts.

However, SKB will limit disposals of cellulose in future waste packages (SKB 2014b) to minimise the potential impact of ISA in 2BMA.

4.2 Gluconate

The sorption of gluconate to hydrated cement conditioning reduces the gluconate concentrations in all cement-conditioned SFR waste packages to between 10^{-10}–10^{-8} M (Table 3-6). Of the remaining three gluconate-containing waste types, B.07 and O.07 are packaged in concrete tanks, which provide sufficient sorption capacity to reduce the gluconate concentrations effectively (Table 3-6). The final waste type, F.17, is packaged in steel and deposited in the BMA. Although the gluconate concentration will not be reduced by the packaging material, dilution and sorption to the hydrated cement in the construction concrete during migration into the relevant BMA compartments are expected to lower the concentration to at least 10^{-9} M (Table 3-7). These concentrations are based on detailed information from the nuclear sites and are therefore likely to be realistic.

4.3 Other complexing agents

NTA was found to have the highest concentration of the other complexing agents in SFR, of up to $2.1 \cdot 10^{-2}$ M inside a waste package, and up to $3.2 \cdot 10^{-3}$ M within a 1BMA compartment. Citrate concentrations also were found to be relatively high, up to $9.8 \cdot 10^{-3}$ M inside a waste package and up to $1.5 \cdot 10^{-3}$ M within a 1BMA compartment (compartment 6). These concentrations are based on detailed information from the nuclear sites and are therefore likely to be realistic for the waste packages, 1BMA, 1 and 2BTF and Silo if the complexing agents are in the solution phase.

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Complexing agents and their potential importance within SFR

Table A-1. Potential complexing agents in SFR and comments on their relevancy and importance for the safety assessment in SFR. This has been adapted from Fanger et al. (2001) who used the 1998 annual environmental report for each plant and interviews with employees in 1998. The new assessments for complexing agents carried out within the current report are underlined and are given in brackets after the 1998 values. NPP= nuclear power plant.

Complexing agent/type of organic material	Source[a]	Comment	Usage/mass to be deposited	Considered
Acetate	Chemicals NPP	Weak complexing agent	Small amounts	No
Acrylates	Chemicals NPP	Relatively strong complexing agent	Possibly used but not identified in SFR	No
Acrylamides	Chemicals NPP	No complexing properties		No
Bitumen degradation products	Waste conditioning; slow degradation under anaerobic conditions	Weak complexing power	Large amounts of bitumen	No
Cellulose degradation products	Clothes, paper, wood etc	Degrades to ISA	See this report	Yes
Citrate	Chemicals NPP	Relatively strong complexing agent (tri-)	1,900 kg (2014 estimate = 320 kg)	Yes
CMC (carboxylmethyl-cellulose)	–	–	Not used	No
Cyanide	Chemicals NPP	Relatively strong complexing agent (ferrocyanides weak)	Small/no amounts	No
DTPA (Diethylene-triamine-pentaacetate)		Strong complexing agent	Not used	No
EDTA (Ethylene-diaminetetra-acetate)	Chemicals NPP	Strong complexing agent	Small amounts, no longer used, ~10 kg	Yes
Ethylacetate	Chemicals NPP	Weak complexing agent	Small amounts	No
Fumarate			Not used	No
Gluconate	Chemicals NPP	Strong complexing agent		Yes
	700 kg (2014 estimate = 680 kg)			
Hydrazine	Corrosion inhibitors	No importance (form H_2, H_2O)	–	No
Inorganic ligands (CO_3^{2-}, NO_3^-, SO_4^{2-}, S^{2-}, PO_4^{3-}, CN^-, $B(OH)_4^-$, F^-, I^-, Cl^-, Br^-)	Chemicals NPP	Little importance	In waste and water	No
Ion-exchange resin degradation products	Waste; radiolytic degradation	Negligible effects	–	No
Lignine, Lignosulphates, lignine sulphonates (Cementa Flyt M97, PA in Betokem)	Cement additives	No longer considered to be cellulosic due to structural differences between lignin and cellulose. This is a change from the assumption used in Fanger et al. (2001)	1,000 kg	No
Maleinic acid (Sikament 10)	Cement additives	See Section 2.3.2	10–12 kg/waste package	No
Methocel	Cement additive in the Silo	Regarded as cellulose = >ISA	5,200 kg	Yes

Complexing agent/type of organic material	Source[a]	Comment	Usage/mass to be deposited	Considered
Melamine formaldehyde (Peramin F and L)	Cement additives	Relatively weak complexing agent	Used, amount not known	No
Methylglycine diacetic acid (MGDA)	Chemicals NPP	Similar to NTA, based on structure and use	Included in NTA estimate	Yes
Nitrite	Chemicals NPP	No importance	Only small amounts	No
NTA (Nitrilotriacetate)	Chemicals NPP	Strong complexing agent (weaker than EDTA and phospho-nates)	800 kg (2014 estimate = 2,700 kg)	Yes
Oxalate/ iron oxalate	Chemicals NPP	Medium strength complexing agent (dicarboxylic)	600 kg/1,200 kg (2014 estimate = 160 kg)	Yes
Phosphate	Chemicals NPP	Strong complexing agent	Used, amounts not known	No
Picolinate	Chemicals NPP	Relatively weak com-plexing agent (one carboxylate group)	3 kg	No
Sodium capryliminodipropionate (NKP)	Chemicals NPP	Not known	310 kg, extrapolating from the amount per O.07 package in 1998 to all packages	Yes
(Tall) fatty acid ("Tallfettsyra")	Chemicals NPP	No longer considered to degrade to ISA. This is a change from the assumption used in Fanger et al. (2001)	15 kg, small amount in comparison to other organic matter	
Tartrate, Alkyl sulphonate, Substituted phenols			Not identified in Fanger et al. 2001	No
UP2 filter aid (polyacrylonitrile) degradation products	Degradation of chemicals NPP	Impact dependent on degradation conditions, see Sec-tion 2.3.2	53,000 kg	No
"Vinsolharts"/ligninesulphonates (Barra 55)	Cement additives	Relatively strong complexing agent	Small amounts	No

[a] Some of the complexing agents may have additional sources to those listed here.

Waste characteristics, distribution of wastes into 1BMA and 2BMA, and characteristics of the repository parts considered

Table B-1. Distribution of waste packages in 1BMA compartments and 2BMA, according to the Initial State Report (SKB 2014b). When only some packages of a certain waste type contain cellulose, the packages containing cellulose have been listed separately and given the suffix "_cell" at the end of the waste package type name; "_C" and "_S" denote concrete and steel packaging when both are possible for a given waste type, while "_FL" and "_FB" show that the packages are grouped in a metal tray or box, respectively.

	1BMA compartment															1BMA total	2BMA total
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15		
B.05_FB			1,168		2,000	192										3,360	
B.05_FL		382	270		96	144										892	
B.23											7	8	8	5	5	33	
B.23D																	486
B.23Dsec																	122
C.01							2			5						7	
C.01_cell				20			10	1	21	9						61	
C.23			1					12	30		7	6	7			63	98
C.4K23D																	3
F.05_1		1,454														1,454	
F_05_2		258														258	
F.15				8		3										11	
F.17						204				211	211	211	212	53	53	1,155	
F.17_cell			144		8	43										195	
F.17_1				20	12											32	
F.23_C				49			2	4		2						57	0
F.23_S				15			10	88		38	21	21	21	3	3	220	250
F.4K23D																	237
F.4K23CD																	70
F.99						2										2	
O.01				11			209	10	28	134	2	1	2			397	
O.01_cell				45			43	19	156	15						278	
O.23				35			36	134	137	113	18	18	18			509	100
O.4K23D																	198
O.4K23CD																	82
O.4K23SD																	15
R.01	576	148	144	144	144	144	144	146	88		2	8	1			1,689	
R.10								36	48		12	12	13			121	
R.15				124							14	14	14	10	10	186	68
R.23_C				124			120	38	52			4				338	
R.23_S								80	16		17	18	17	12	12	172	96
R.23D																	153
R.4K23D																	314
R.4K23CD																	149
R.29											64	60	64			188	192
S.21											110	110	110	79	79	488	
S.23											39	35	39			113	605
S.23D																	164
S.25D																	2,384
Å.4K23D																	45
Å.4K23CD																	5

Table B-2. Mass (kg) of cellulose and complexing agents in the 1BMA compartments, 1BMA, 2BMA, the Silo and 1 and 2BTF.

	Cellulose	Sodium gluconate	EDTA	NKP	NTA	Citrate	Oxalate
1BMA compartment							
1							
2							
3	619	10	1.0		99	46	2.4
4	7,450	16	0.4		138		
5	34	2.0	0.2		19	9	0.5
6	185	18	1.8		179	83	4.4
7	5,040		0.0				
8	22,000	4.8	0.1		41		
9	9,910	6.4	0.1		55		
10	9,640	2.9	0.3		28	13	0.7
11	6,960	4.6	0.4		44	18	1.0
12	6,940	3.4	0.3		33	13	0.7
13	7,000	3.4	0.3		33	13	0.7
14	1,820	0.5	0.0		4		
15	1,820	0.5	0.0		4		
Total 1BMA	79,500	73	5.0		679	195	10
Total 2BMA	70,600						
Total Silo	23,200*	184	1.9		1,590		90
Total 1 and 2BTF	1,070+	401	5.0	308	262	69	

*Includes 5,200 kg of Methocel cement additive. +Only present in 1BTF.

Table B-3. Characteristics of the waste packages that contain either cellulose or complexing agents. "_C" and "_S" denote concrete and steel packaging when both are possible for a given waste type.

			Hydrated cement, kg			Pore and void volumes, m³				
Vault	Waste type	Conditioning	Waste and conditioning	Pack-aging	Total: entire package	Void volume	Pore volume in waste and conditioning	Pore volume in packaging	Total pore and void: inside packaging	Total pore and void: entire package
1 and 2BMA	B.23	Concrete	516	102*	618	0.430	0.161	0.030*	0.591	0.621
	B.23Dsec	Concrete	516	102*	618	0.430	0.161	0.030*	0.591	0.621
	C.01	Cement	1,540	375	1,915	0.330	0.101	0.109	0.431	0.540
	C.23	Concrete	215	375	590	0.250	0.113	0.109	0.363	0.472
	F.17	Bitumen	0	0	0	0.170	0	0	0.170	0.170
	F.23_C	Concrete	215	375	590	0.250	0.113	0.109	0.363	0.472
	F.23_S	Concrete	516	102*	618	0.430	0.161	0.030*	0.591	0.621
	O.01	Cement	1,540	375	1,915	0.330	0.101	0.109	0.431	0.540
	O.23	Concrete	215	375	590	0.250	0.113	0.109	0.363	0.472
	R.10	Cement	1,120	375	1,495	0.330	0.101	0.109	0.431	0.540
	R.15	Cement	2,100	102*	2,202	0.085	0.213	0.030*	0.298	0.327
	R.23_C	Concrete	215	375	590	0.250	0.113	0.109	0.363	0.472
	R.23_S	Concrete	516	102*	618	0.430	0.161	0.030*	0.591	0.621
	S.21	Concrete	37	0	37	0.011	0.015	0	0.026	0.026
	S.23	Concrete	215	375	590	0.067	0.140	0.109	0.207	0.316
Silo	B.04	Cement	75	0	75	0.024	0.032	0	0.056	0.056
	C.02	Cement	586	375	961	0.330	0.101	0.109	0.431	0.540
	C.24	Concrete	381	375	755	0.250	0.113	0.109	0.363	0.472
	O.02	Cement	586	375	961	0.330	0.101	0.109	0.431	0.540
	R.16	Cement	799	102*	901	0.085	0.213	0.030*	0.298	0.327
	O.24	Concrete	560	0	560	0.430	0.086	0	0.516	0.516
	R.24	Concrete	560	0	560	0.430	0.191	0	0.621	0.621
	S.11	Cement	693	0	693	0.085	0.242	0	0.327	0.327
	S.24_C	Concrete	267	375	641	0.250	0.113	0.109	0.363	0.472
	S.24_S	Concrete	560	0	560	0.430	0.086	0	0.516	0.516
1 and 2BTF	B.07	Dewatering	0	1,990	1,990	0.500	2.200	0.580	2.700	3.280
	O.07	Dewatering	0	1,990	1,990	1.000	2.000	0.580	3.000	3.580
	O.99:1	Cement	2,795	0	2,795	0.180	0.572	0	0.752	0.752
	R.23_C	Concrete	215	375	590	0.250	0.113	0.109	0.363	0.472

* Steel packaging with concrete lid.

Table B-4. Pore volumes and masses of hydrated cement in the specified units of SFR.

	Hydrated cement, kg				Pore and void volume, m³			
	Waste packages	Construction concrete	Grout	Total	Waste packages	Construction concrete	Grout	Total
1BMA compartment								
1	$1.02 \cdot 10^6$	$1.63 \cdot 10^5$	$5.23 \cdot 10^4$	$1.24 \cdot 10^6$	$3.11 \cdot 10^2$	$4.76 \cdot 10^1$	$2.27 \cdot 10^1$	$3.81 \cdot 10^2$
2	$2.63 \cdot 10^5$	$1.50 \cdot 10^5$	$1.64 \cdot 10^5$	$5.76 \cdot 10^5$	$2.38 \cdot 10^2$	$4.37 \cdot 10^1$	$7.11 \cdot 10^1$	$3.52 \cdot 10^2$
3	$2.56 \cdot 10^5$	$1.50 \cdot 10^5$	$1.20 \cdot 10^5$	$5.25 \cdot 10^5$	$2.53 \cdot 10^2$	$4.37 \cdot 10^1$	$5.21 \cdot 10^1$	$3.49 \cdot 10^2$
4	$8.13 \cdot 10^5$	$1.50 \cdot 10^5$	$5.23 \cdot 10^4$	$1.02 \cdot 10^6$	$2.70 \cdot 10^2$	$4.37 \cdot 10^1$	$2.27 \cdot 10^1$	$3.37 \cdot 10^2$
5	$2.56 \cdot 10^5$	$1.50 \cdot 10^5$	$1.73 \cdot 10^5$	$5.78 \cdot 10^5$	$2.46 \cdot 10^2$	$4.37 \cdot 10^1$	$7.52 \cdot 10^1$	$3.65 \cdot 10^2$
6	$2.59 \cdot 10^5$	$1.50 \cdot 10^5$	$1.78 \cdot 10^5$	$5.86 \cdot 10^5$	$1.75 \cdot 10^2$	$4.37 \cdot 10^1$	$7.71 \cdot 10^1$	$2.96 \cdot 10^2$
7	$8.60 \cdot 10^5$	$1.50 \cdot 10^5$	$5.23 \cdot 10^4$	$1.06 \cdot 10^6$	$3.01 \cdot 10^2$	$4.37 \cdot 10^1$	$2.27 \cdot 10^1$	$3.67 \cdot 10^2$
8	$5.85 \cdot 10^5$	$1.50 \cdot 10^5$	$6.19 \cdot 10^4$	$7.97 \cdot 10^5$	$3.07 \cdot 10^2$	$4.37 \cdot 10^1$	$2.69 \cdot 10^1$	$3.78 \cdot 10^2$
9	$7.59 \cdot 10^5$	$1.50 \cdot 10^5$	$5.23 \cdot 10^4$	$9.61 \cdot 10^5$	$2.97 \cdot 10^2$	$4.37 \cdot 10^1$	$2.27 \cdot 10^1$	$3.64 \cdot 10^2$
10	$4.03 \cdot 10^5$	$1.50 \cdot 10^5$	$1.11 \cdot 10^5$	$6.64 \cdot 10^5$	$2.02 \cdot 10^2$	$4.37 \cdot 10^1$	$4.81 \cdot 10^1$	$2.93 \cdot 10^2$
11	$2.52 \cdot 10^5$	$1.50 \cdot 10^5$	$2.27 \cdot 10^5$	$6.29 \cdot 10^5$	$1.41 \cdot 10^2$	$4.37 \cdot 10^1$	$9.87 \cdot 10^1$	$2.83 \cdot 10^2$
12	$2.54 \cdot 10^5$	$1.50 \cdot 10^5$	$2.25 \cdot 10^5$	$6.28 \cdot 10^5$	$1.43 \cdot 10^2$	$4.37 \cdot 10^1$	$9.77 \cdot 10^1$	$2.84 \cdot 10^2$
13	$2.52 \cdot 10^5$	$1.50 \cdot 10^5$	$2.25 \cdot 10^5$	$6.27 \cdot 10^5$	$1.41 \cdot 10^2$	$4.37 \cdot 10^1$	$9.77 \cdot 10^1$	$2.83 \cdot 10^2$
14	$3.73 \cdot 10^4$	$6.17 \cdot 10^4$	$6.78 \cdot 10^4$	$1.67 \cdot 10^5$	$2.83 \cdot 10^1$	$1.80 \cdot 10^1$	$2.94 \cdot 10^1$	$7.57 \cdot 10^1$
15	$3.73 \cdot 10^4$	$6.17 \cdot 10^4$	$6.78 \cdot 10^4$	$1.67 \cdot 10^5$	$2.83 \cdot 10^1$	$1.80 \cdot 10^1$	$2.94 \cdot 10^1$	$7.57 \cdot 10^1$
Total in compartments	$6.31 \cdot 10^6$	$2.08 \cdot 10^6$	$1.83 \cdot 10^6$	$1.02 \cdot 10^7$	$3.08 \cdot 10^3$	$6.07 \cdot 10^2$	$7.94 \cdot 10^2$	$4.48 \cdot 10^3$
Total in 1BMA vault	$6.31 \cdot 10^6$	$2.12 \cdot 10^6$	$2.11 \cdot 10^{6*}$	$1.05 \cdot 10^7$	$3.08 \cdot 10^3$	$6.19 \cdot 10^2$	$2.77 \cdot 10^{5+}$	$1.49 \cdot 10^4$
2BMA								
2BMA caisson (dividing waste into 8.4 caissons)	$7.28 \cdot 10^5$	$2.55 \cdot 10^5$	$1.67 \cdot 10^5$	$1.15 \cdot 10^6$	$4.77 \cdot 10^2$	$7.42 \cdot 10^1$	$6.50 \cdot 10^1$	$6.16 \cdot 10^2$
Silo								
Silo (inside outer walls)	$7.23 \cdot 10^6$	$2.84 \cdot 10^6$	$3.84 \cdot 10^6$	$1.39 \cdot 10^7$	$4.02 \cdot 10^3$	$8.28 \cdot 10^2$	$1.67 \cdot 10^3$	$6.50 \cdot 10^3$
Silo construction	$7.23 \cdot 10^6$	$5.21 \cdot 10^6$	$3.84 \cdot 10^6$	$1.63 \cdot 10^7$	$4.02 \cdot 10^3$	$1.52 \cdot 10^3$	$1.67 \cdot 10^3$	$7.21 \cdot 10^3$
Silo vault	$7.23 \cdot 10^6$	$5.32 \cdot 10^6$	$3.84 \cdot 10^{6*}$	$1.64 \cdot 10^7$	$4.02 \cdot 10^3$	$1.52 \cdot 10^3$	$7.02 \cdot 10^{3+}$	$1.25 \cdot 10^4$
1 and 2BTF								
1BTF waste zone	$3.08 \cdot 10^6$	$1.03 \cdot 10^6$	$1.64 \cdot 10^6$	$5.75 \cdot 10^6$	$1.84 \cdot 10^3$	$3.00 \cdot 10^2$	$9.33 \cdot 10^2$	$3.07 \cdot 10^3$
1BTF vault	$3.08 \cdot 10^6$	$1.08 \cdot 10^6$	$1.82 \cdot 10^{6*}$	$5.98 \cdot 10^6$	$1.84 \cdot 10^3$	$3.16 \cdot 10^2$	$4.25 \cdot 10^{3+}$	$6.40 \cdot 10^3$
2BTF waste zone	$1.58 \cdot 10^6$	$1.03 \cdot 10^6$	$1.06 \cdot 10^6$	$3.67 \cdot 10^6$	$2.59 \cdot 10^3$	$3.00 \cdot 10^2$	$6.03 \cdot 10^2$	$3.49 \cdot 10^3$
2BTF vault	$1.58 \cdot 10^6$	$1.08 \cdot 10^6$	$1.24 \cdot 10^{6*}$	$3.90 \cdot 10^6$	$2.59 \cdot 10^3$	$3.16 \cdot 10^2$	$3.92 \cdot 10^{3+}$	$6.82 \cdot 10^3$

* Includes shotcrete. + Includes shotcrete, macadam and unfilled space at the top of the vault.

Table B-5. Distribution of the BMA waste packages that contain complexing agents between the 1BMA compartments.

1BMA compartment	F.17	R.10	R.15
1			
2			
3	144		
4			124
5	28		
6	259		
7			
8		36	
9		48	
10	41		
11	56		5
12	40		5
13	40		5
14			4
15			4
Total	608	84	147

Additional concentration data for different time periods (ISA) or in different units of SFR

Table C-1. ISA concentrations (M) inside the waste packages as a function of time. Sorption of ISA to available hydrated cement has been taken into account and concentrations that are more than twice the solubility limit for α-ISA during the portlandite phase of cement degradation (0.02 M), i.e. 0.04 M, are given in brackets.

| | Time (years) | | | | |
	10	100	500	1,000	5,000
1 and 2BMA					
B.23	$9.9 \cdot 10^{-5}$	$4.1 \cdot 10^{-4}$	$1.6 \cdot 10^{-2}$	$(5.3 \cdot 10^{-2})$	$(1.5 \cdot 10^{-1})$
B.23Dsec	$9.9 \cdot 10^{-5}$	$4.1 \cdot 10^{-4}$	$1.6 \cdot 10^{-2}$	$(5.3 \cdot 10^{-2})$	$(1.5 \cdot 10^{-1})$
C.01_cell	$1.4 \cdot 10^{-5}$	$4.0 \cdot 10^{-5}$	$1.6 \cdot 10^{-4}$	$3.1 \cdot 10^{-4}$	$7.6 \cdot 10^{-4}$
C.23	$1.8 \cdot 10^{-4}$	$1.1 \cdot 10^{-3}$	$(4.4 \cdot 10^{-2})$	$(1.0 \cdot 10^{-1})$	$(2.3 \cdot 10^{-1})$
F.17_cell	$4.4 \cdot 10^{-3}$	$1.3 \cdot 10^{-2}$	$(4.2 \cdot 10^{-2})$	$(6.7 \cdot 10^{-2})$	$(1.1 \cdot 10^{-1})$
F.23C	$1.7 \cdot 10^{-4}$	$1.0 \cdot 10^{-3}$	$(4.1 \cdot 10^{-2})$	$(9.8 \cdot 10^{-2})$	$(2.2 \cdot 10^{-1})$
F.23S	$5.6 \cdot 10^{-4}$	$1.7 \cdot 10^{-2}$	$(2.3 \cdot 10^{-1})$	$(4.6 \cdot 10^{-1})$	$(8.9 \cdot 10^{-1})$
O.01_cell	$1.4 \cdot 10^{-5}$	$4.0 \cdot 10^{-5}$	$1.6 \cdot 10^{-4}$	$3.1 \cdot 10^{-4}$	$7.6 \cdot 10^{-4}$
O.23	$1.8 \cdot 10^{-4}$	$1.1 \cdot 10^{-3}$	$(4.4 \cdot 10^{-2})$	$(1.0 \cdot 10^{-1})$	$(2.3 \cdot 10^{-1})$
R.23C	$5.6 \cdot 10^{-5}$	$1.9 \cdot 10^{-4}$	$2.0 \cdot 10^{-3}$	$1.2 \cdot 10^{-2}$	$(4.1 \cdot 10^{-2})$
R.23S	$9.9 \cdot 10^{-5}$	$4.1 \cdot 10^{-4}$	$1.6 \cdot 10^{-2}$	$(5.3 \cdot 10^{-2})$	$(1.5 \cdot 10^{-1})$
S.21	$3.4 \cdot 10^{-4}$	$6.3 \cdot 10^{-3}$	$2.0 \cdot 10^{-1}$	$4.6 \cdot 10^{-1}$	$9.6 \cdot 10^{-1}$
S.23	$1.7 \cdot 10^{-4}$	$1.0 \cdot 10^{-3}$	$5.8 \cdot 10^{-2}$	$1.5 \cdot 10^{-1}$	$3.7 \cdot 10^{-1}$
Silo					
C.24	$1.1 \cdot 10^{-4}$	$4.6 \cdot 10^{-4}$	$2.2 \cdot 10^{-2}$	$(7.0 \cdot 10^{-2})$	$(1.9 \cdot 10^{-1})$
O.24	$9.0 \cdot 10^{-6}$	$2.6 \cdot 10^{-5}$	$9.9 \cdot 10^{-5}$	$1.7 \cdot 10^{-4}$	$3.6 \cdot 10^{-4}$
R.24	$9.0 \cdot 10^{-6}$	$2.6 \cdot 10^{-5}$	$9.8 \cdot 10^{-5}$	$1.7 \cdot 10^{-4}$	$3.6 \cdot 10^{-4}$
S.11	$4.4 \cdot 10^{-6}$	$1.3 \cdot 10^{-5}$	$4.4 \cdot 10^{-5}$	$7.4 \cdot 10^{-5}$	$1.3 \cdot 10^{-4}$
S.24C	$1.9 \cdot 10^{-5}$	$5.8 \cdot 10^{-5}$	$2.5 \cdot 10^{-4}$	$5.3 \cdot 10^{-4}$	$1.8 \cdot 10^{-3}$
S.24S	$9.0 \cdot 10^{-6}$	$2.6 \cdot 10^{-5}$	$9.9 \cdot 10^{-5}$	$1.7 \cdot 10^{-4}$	$3.6 \cdot 10^{-4}$
1BTF					
O.99:1	$7.6 \cdot 10^{-6}$	$2.2 \cdot 10^{-5}$	$8.1 \cdot 10^{-5}$	$1.4 \cdot 10^{-4}$	$2.8 \cdot 10^{-4}$
R.23	$5.6 \cdot 10^{-5}$	$1.9 \cdot 10^{-4}$	$2.0 \cdot 10^{-3}$	$1.2 \cdot 10^{-2}$	$(4.1 \cdot 10^{-2})$

Table C-2. ISA concentrations (M) in the waste packages, including the packaging material as a function of time. Sorption of ISA to available hydrated cement has been taken into account and concentrations that are more than twice the solubility limit for α-ISA during the portlandite phase of cement degradation (0.02 M), i.e. 0.04 M, are given in brackets.

| | Time (years) | | | | |
	10	100	500	1,000	5,000
1BMA and 2BMA					
B.23	$8.1 \cdot 10^{-5}$	$3.1 \cdot 10^{-4}$	$8.7 \cdot 10^{-3}$	$(3.7 \cdot 10^{-2})$	$(1.1 \cdot 10^{-1})$
B.23Dsec	$8.1 \cdot 10^{-5}$	$3.1 \cdot 10^{-4}$	$8.7 \cdot 10^{-3}$	$(3.7 \cdot 10^{-2})$	$(1.1 \cdot 10^{-1})$
C.01_cell	$1.1 \cdot 10^{-5}$	$3.2 \cdot 10^{-5}$	$1.2 \cdot 10^{-4}$	$2.2 \cdot 10^{-4}$	$4.9 \cdot 10^{-4}$
C.23	$5.6 \cdot 10^{-5}$	$1.9 \cdot 10^{-4}$	$2.1 \cdot 10^{-3}$	$1.5 \cdot 10^{-2}$	$(6.3 \cdot 10^{-2})$
F.17_cell	$4.4 \cdot 10^{-3}$	$1.3 \cdot 10^{-2}$	$(4.2 \cdot 10^{-2})$	$(6.7 \cdot 10^{-2})$	$(1.1 \cdot 10^{-1})$
F.23C	$5.4 \cdot 10^{-5}$	$1.8 \cdot 10^{-4}$	$1.9 \cdot 10^{-3}$	$1.3 \cdot 10^{-2}$	$(5.8 \cdot 10^{-2})$
F.23S	$4.1 \cdot 10^{-4}$	$9.5 \cdot 10^{-3}$	$(1.9 \cdot 10^{-1})$	$(4.0 \cdot 10^{-1})$	$(8.1 \cdot 10^{-1})$
O.01_cell	$1.1 \cdot 10^{-5}$	$3.2 \cdot 10^{-5}$	$1.2 \cdot 10^{-4}$	$2.2 \cdot 10^{-4}$	$4.9 \cdot 10^{-4}$
O.23	$5.6 \cdot 10^{-5}$	$1.9 \cdot 10^{-4}$	$2.1 \cdot 10^{-3}$	$1.5 \cdot 10^{-2}$	$(6.3 \cdot 10^{-2})$
R.23C	$1.9 \cdot 10^{-5}$	$5.8 \cdot 10^{-5}$	$2.5 \cdot 10^{-4}$	$5.3 \cdot 10^{-4}$	$1.9 \cdot 10^{-3}$
R.23S	$8.1 \cdot 10^{-5}$	$3.1 \cdot 10^{-4}$	$8.7 \cdot 10^{-3}$	$(3.7 \cdot 10^{-2})$	$(1.1 \cdot 10^{-1})$
S.21	$3.4 \cdot 10^{-4}$	$6.3 \cdot 10^{-3}$	$(2.0 \cdot 10^{-1})$	$(4.6 \cdot 10^{-1})$	$(9.6 \cdot 10^{-1})$
S.23	$5.4 \cdot 10^{-5}$	$1.8 \cdot 10^{-4}$	$1.9 \cdot 10^{-3}$	$1.5 \cdot 10^{-2}$	$(7.1 \cdot 10^{-2})$
Silo					
C.24	$5.0 \cdot 10^{-5}$	$1.7 \cdot 10^{-4}$	$1.6 \cdot 10^{-3}$	$1.1 \cdot 10^{-2}$	$(5.7 \cdot 10^{-2})$
O.24	$9.0 \cdot 10^{-6}$	$2.6 \cdot 10^{-5}$	$9.9 \cdot 10^{-5}$	$1.7 \cdot 10^{-4}$	$3.6 \cdot 10^{-4}$
R.24	$9.0 \cdot 10^{-6}$	$2.6 \cdot 10^{-5}$	$9.8 \cdot 10^{-5}$	$1.7 \cdot 10^{-4}$	$3.6 \cdot 10^{-4}$
S.11	$4.4 \cdot 10^{-6}$	$1.3 \cdot 10^{-5}$	$4.4 \cdot 10^{-5}$	$7.4 \cdot 10^{-5}$	$1.3 \cdot 10^{-4}$
S.24C	$7.9 \cdot 10^{-6}$	$2.3 \cdot 10^{-5}$	$8.4 \cdot 10^{-5}$	$1.5 \cdot 10^{-4}$	$2.9 \cdot 10^{-4}$
S.24S	$9.0 \cdot 10^{-6}$	$2.6 \cdot 10^{-5}$	$9.9 \cdot 10^{-5}$	$1.7 \cdot 10^{-4}$	$3.6 \cdot 10^{-4}$
1BTF					
O.99:1	$7.6 \cdot 10^{-6}$	$2.2 \cdot 10^{-5}$	$8.1 \cdot 10^{-5}$	$1.4 \cdot 10^{-4}$	$2.8 \cdot 10^{-4}$
R.23	$1.9 \cdot 10^{-5}$	$5.8 \cdot 10^{-5}$	$2.5 \cdot 10^{-4}$	$5.3 \cdot 10^{-4}$	$1.9 \cdot 10^{-3}$

Table C-3. Concentrations of ISA (M) over time for each relevant unit of SFR, based on the degradation of cellulose after 5,000 years and considering sorption to all available hydrated cement.

	Time (years)				
	10	100	500	1,000	5,000
1BMA: compartment					
1	0	0	0	0	0
2	0	0	0	0	0
3	$1.2 \cdot 10^{-6}$	$3.4 \cdot 10^{-6}$	$1.1 \cdot 10^{-5}$	$1.8 \cdot 10^{-5}$	$3.1 \cdot 10^{-5}$
4	$7.4 \cdot 10^{-6}$	$2.2 \cdot 10^{-5}$	$7.9 \cdot 10^{-5}$	$1.4 \cdot 10^{-4}$	$2.7 \cdot 10^{-4}$
5	$5.9 \cdot 10^{-8}$	$1.7 \cdot 10^{-7}$	$5.6 \cdot 10^{-7}$	$9.0 \cdot 10^{-7}$	$1.5 \cdot 10^{-6}$
6	$3.2 \cdot 10^{-7}$	$9.0 \cdot 10^{-7}$	$3.0 \cdot 10^{-6}$	$4.8 \cdot 10^{-6}$	$8.0 \cdot 10^{-6}$
7	$4.8 \cdot 10^{-6}$	$1.4 \cdot 10^{-5}$	$4.9 \cdot 10^{-5}$	$8.2 \cdot 10^{-5}$	$1.5 \cdot 10^{-4}$
8	$2.9 \cdot 10^{-5}$	$9.1 \cdot 10^{-5}$	$4.7 \cdot 10^{-4}$	$1.3 \cdot 10^{-3}$	$1.2 \cdot 10^{-2}$
9	$1.0 \cdot 10^{-5}$	$3.1 \cdot 10^{-5}$	$1.2 \cdot 10^{-4}$	$2.1 \cdot 10^{-4}$	$4.6 \cdot 10^{-4}$
10	$1.5 \cdot 10^{-5}$	$4.4 \cdot 10^{-5}$	$1.8 \cdot 10^{-4}$	$3.5 \cdot 10^{-4}$	$9.2 \cdot 10^{-4}$
11	$1.1 \cdot 10^{-5}$	$3.3 \cdot 10^{-5}$	$1.3 \cdot 10^{-4}$	$2.3 \cdot 10^{-4}$	$5.2 \cdot 10^{-4}$
12	$1.1 \cdot 10^{-5}$	$3.3 \cdot 10^{-5}$	$1.3 \cdot 10^{-4}$	$2.3 \cdot 10^{-4}$	$5.2 \cdot 10^{-4}$
13	$1.1 \cdot 10^{-5}$	$3.4 \cdot 10^{-5}$	$1.3 \cdot 10^{-4}$	$2.4 \cdot 10^{-4}$	$5.3 \cdot 10^{-4}$
14	$1.1 \cdot 10^{-5}$	$3.3 \cdot 10^{-5}$	$1.3 \cdot 10^{-4}$	$2.3 \cdot 10^{-4}$	$5.1 \cdot 10^{-4}$
15	$1.1 \cdot 10^{-5}$	$3.3 \cdot 10^{-5}$	$1.3 \cdot 10^{-4}$	$2.3 \cdot 10^{-4}$	$5.1 \cdot 10^{-4}$
Total 1BMA construction	$7.9 \cdot 10^{-6}$	$2.3 \cdot 10^{-5}$	$8.4 \cdot 10^{-5}$	$1.5 \cdot 10^{-4}$	$2.9 \cdot 10^{-4}$
1BMA vault incl. macadam and shotcrete	$7.6 \cdot 10^{-6}$	$2.2 \cdot 10^{-5}$	$8.1 \cdot 10^{-5}$	$1.4 \cdot 10^{-4}$	$2.7 \cdot 10^{-4}$
2BMA					
2BMA per caisson (8.4 caisson)	$7.4 \cdot 10^{-6}$	$2.2 \cdot 10^{-5}$	$7.9 \cdot 10^{-5}$	$1.4 \cdot 10^{-4}$	$2.6 \cdot 10^{-4}$
Silo					
Within the outer walls of the Silo construction	$1.7 \cdot 10^{-6}$	$4.8 \cdot 10^{-6}$	$1.6 \cdot 10^{-5}$	$2.6 \cdot 10^{-5}$	$4.5 \cdot 10^{-5}$
Silo construction	$1.4 \cdot 10^{-6}$	$4.1 \cdot 10^{-6}$	$1.4 \cdot 10^{-5}$	$2.2 \cdot 10^{-5}$	$3.8 \cdot 10^{-5}$
Entire vault	$1.4 \cdot 10^{-6}$	$4.0 \cdot 10^{-6}$	$1.4 \cdot 10^{-5}$	$2.2 \cdot 10^{-5}$	$3.8 \cdot 10^{-5}$
1BTF					
Waste zone	$1.9 \cdot 10^{-7}$	$5.3 \cdot 10^{-7}$	$1.8 \cdot 10^{-6}$	$2.8 \cdot 10^{-6}$	$4.7 \cdot 10^{-6}$
Entire vault	$1.8 \cdot 10^{-7}$	$5.1 \cdot 10^{-7}$	$1.7 \cdot 10^{-6}$	$2.7 \cdot 10^{-6}$	$4.5 \cdot 10^{-6}$

Table C-4. Complexing agent concentrations in the waste packages, including the waste packaging material. Note that: O.07 and B.07 show the maximum concentration of each complexing agent identified in either 1998 or the recent assessment. Oxalate concentrations that exceed the solubility limit expected under repository conditions, 10^{-5} M, are given in brackets.

	Concentration (M)				
	EDTA	NKP	NTA	Citrate	Oxalate
BMA					
F.17	$1.4 \cdot 10^{-4}$		$2.1 \cdot 10^{-2}$	$9.8 \cdot 10^{-3}$	$(1.1 \cdot 10^{-3})$
R.10	$1.8 \cdot 10^{-5}$		$1.1 \cdot 10^{-2}$		
R.15	$3.0 \cdot 10^{-5}$		$1.8 \cdot 10^{-2}$		
Silo					
B.04					$(2.3 \cdot 10^{-2})$
C.02			$6.6 \cdot 10^{-4}$		
O.02					$(3.0 \cdot 10^{-3})$
R.16	$3.0 \cdot 10^{-5}$		$1.7 \cdot 10^{-2}$		
BTF					
B.07	$1.4 \cdot 10^{-5}$		$5.5 \cdot 10^{-7}$	$4.0 \cdot 10^{-4}$	
O.07	$6.0 \cdot 10^{-6}$	$7.1 \cdot 10^{-4}$	$2.3 \cdot 10^{-3}$	$5.8 \cdot 10^{-5}$	