

Preparatory Safety Assessment

Conceptual model description of the reference case

Authors:

Eef Weetjens, Jan Marivoet and Joan Govaerts

Editor:

Bertrand Leterme

**NIRAS/ONDRAF Contract CCHO – 2009-00940000
Research Plan SAF**

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Contents

Contents.....	5
1 Introduction.....	7
1.1 Context and objective.....	7
1.2 The Safety strategy.....	8
1.2.1 Overview.....	8
1.2.2 The safety concept.....	10
1.2.3 The disposal system and its environment.....	11
1.2.4 The safety functions.....	12
1.3 Methodology for safety assessments in the SFC1 framework.....	14
1.3.1 Overview.....	14
1.3.2 Methodology for the treatment of parameter uncertainty.....	16
1.4 Scope of this document.....	17
2 Radioactive waste specifications.....	18
2.1 Belgian waste categories.....	18
2.2 Spent fuel management scenarios and waste volumes.....	19
2.2.1 Waste volumes due to electricity production.....	19
2.2.2 Historical waste volumes.....	21
2.3 Radionuclide inventories.....	21
2.3.1 UOX spent fuel.....	21
2.3.2 MOX spent fuel.....	22
2.3.3 Vitrified high-level waste (CSD-V canisters).....	23
2.3.4 Compacted waste (CSD-C canisters).....	23
2.4 Type and characteristics of the primary waste packages.....	24
2.4.1 UOX spent fuel.....	24
2.4.2 MOX spent fuel.....	25
2.4.3 Vitrified HLW (CSD-V canister).....	25
2.4.4 Compacted waste (CSD-C canister).....	25
3 Host formation and reference repository design for Category B&C waste.....	27
3.1 Engineered barrier design.....	27
3.1.1 The supercontainer.....	27
3.1.2 The monolith.....	29
3.2 Repository design.....	30
3.3 Geological host formation and surrounding geological layers.....	31
4 The reference scenario.....	37
4.1 Definition of the reference scenario.....	37
4.2 Exposure pathways.....	37
4.3 Safety and Performance Indicators.....	38
4.4 Phenomenological evolution of the disposal system.....	39
4.4.1 Thermal evolution.....	40
4.4.2 Hydromechanical evolution.....	44
4.4.3 Chemical evolution.....	45
4.4.4 Biological evolution.....	50
4.4.5 Radiological evolution.....	51
4.4.6 Summary: reference evolution in performance assessment.....	51
4.5 Evolution of the environment of the disposal system.....	52
5 The reference case.....	54
5.1 Conceptual model.....	54
5.1.1 Isolation (I).....	54

5.1.2	Engineered containment (C).....	54
5.1.3	Limitation of radionuclide releases (R1).....	56
5.1.4	Limitation of water flow (R2).....	61
5.1.5	Retardation and spreading in time of radionuclide migration (R3).....	62
5.1.6	Dilution in aquifer systems.....	66
5.1.7	Radionuclide transport in the biosphere.....	72
5.2	Mathematical model.....	73
5.2.1	Domain and geometry.....	73
5.2.2	Governing transport equations.....	74
5.2.3	Transport equations of actinide decay chains.....	74
5.2.4	Reaction rate (precipitation/dissolution).....	75
5.2.5	Dissolved Organic Matter (DOM) facilitated transport.....	75
5.2.6	Calculation of safety and performance indicators.....	77
6	Iterations of the reference case.....	79
6.1	Version 1.....	80
6.2	Version 2.....	81
6.2.1	NOM-linked radionuclide transport.....	81
6.2.2	Engineered containment.....	82
6.2.3	Spent fuel matrix dissolution.....	82
6.2.4	Other refinements.....	82
6.3	Version 3.....	83
6.4	Version 4.....	83
7	References.....	84
Annex:	Selection of radionuclides to be considered in the reference case.....	91
A1	Fission and activation products.....	91
A2	Actinide chains.....	93

1 Introduction

1.1 Context and objective

The Belgian radioactive waste management organisation, ONDRAF/NIRAS, is responsible for developing a safe solution for the management of Belgian radioactive waste in the long term. The reference solution adopted for long term management of Category B waste (*i.e.*, low-level and intermediate-level long-lived radioactive waste (LILW-LL)) and Category C waste (*i.e.*, vitrified high-level radioactive waste (HLW) and spent nuclear fuel) is geological disposal in a stable and suitable host formation. The Boom Clay formation is the reference host formation, while the Ypresian Clay formation is considered as an alternative. Studies for over 30 years show that the characteristics of Boom Clay, a low permeable plastic clay layer, are promising for hosting such a geological repository. Most of the information related to the Boom Clay comes from the underground research laboratory HADES, located beneath the Mol-Dessel region in north-east Belgium. This region also serves as a reference site for methodological research associated with the Category B and C waste disposal programme.

The principal objective of any facility for the disposal of radioactive waste is to provide long-term safety by protecting humans and the environment from the harmful effects of ionising radiation. The commonly adopted management strategy to achieve this objective is to concentrate and contain the waste and to isolate it from the biosphere. This strategy forms the starting point for the design of the Belgian safety concept for geological disposal.

ONDRAF/NIRAS is preparing its first Safety and Feasibility Case (SFC1) to demonstrate the long-term safety of its deep disposal concept for Category B and C wastes. A safety case includes the assessment basis, an overall description of the disposal system, and a description of the scientific and technical data and understanding relevant to the assessment of system safety and feasibility (NEA, 2004). Specifically, SFC1 is a decision-oriented document assessing the safety and feasibility of a geological repository for disposal of category C (heat-emitting) and B (long-lived) wastes in the considered argillaceous formations (Boom Clay and Ypresian Clay). The objective of SFC1 is to demonstrate that for the considered zones and for all currently foreseeable B&C waste classes there are no uncertainties that can call into question the capacity of the disposal system to fulfill its requirements and that it is therefore expected to ensure passive safety, while being feasible (ONDRAF/NIRAS, 2009b).

The SFC1 is based on a safety strategy developed to conceptualise and design a geological disposal system that can meet the objectives of passive long-term safety and feasibility. The safety strategy led to the development of a set of safety functions and of safety concepts for the main category B&C waste classes (ONDRAF/NIRAS, 2009a). A new safety assessment methodology has also been developed (ONDRAF/NIRAS, 2009c).

In the context of SFC1, the objective of the present report is to provide a first tentative definition of the reference scenario and reference case for a hypothetical geological repository of B&C waste in Boom Clay at the reference site Mol-Dessel. The main part of the reference scenario consists of a description of the reference evolution of the disposal system and its environment. The reference case can be considered the most simple, robust and defensible conceptual representation of the reference evolution that still upholds the safety concept. It is iteratively developed and tested using limiting values of the expert range. In this report, the description of

the reference case is limited to the conceptual model description of the corresponding performance assessment model, that was tested and applied in versions 1 to 3 (see Chapter 6 for more information on the subsequent iterations of the reference case). Therefore, this report involves little discussion on parameter values because the process for data selection and the data themselves are still being iteratively refined in the current stage of preparatory safety assessment (PSA). The PSA development work builds on previous formal assessments (notably the SAFIR 2 report; ONDRAF/NIRAS, 2001), and uses the design, additional knowledge acquired during assessment basis development and the performance assessment analysis toolbox as input. The validity of the conceptual model descriptions of processes taken into account in the reference case and their application domain were verified with key experts during a 4-day workshop held in October 2011 (see MoM's by Pirot, 2012).

1.2 The Safety strategy

1.2.1 Overview

Following the SAFIR 2 review, the NEA International Review Team advised ONDRAF/NIRAS to develop the frame and tools to embed its national programme in a societal dialogue and in a stepwise decision-making plan with key milestones stretching over the next decades towards the licensing process. ONDRAF/NIRAS has reassessed the organization of its geological disposal programme to serve these ends, and has worked out a safety and feasibility strategy (ONDRAF/NIRAS, 2009a; and subsequent revisions in ONDRAF/NIRAS, to be published). The strategy, illustrated in Figure 1, sets out in broad terms how it is envisaged that safe disposal will be achieved. It includes boundary conditions to be met, strategic choices to be made, requirements to be satisfied and safety principles to be applied. Boundary conditions include, for example, the relevant international and national regulatory framework, institutional policy and conditions required by other stakeholders. Furthermore, a number of high-level strategic choices were made by ONDRAF/NIRAS in order to focus the geological disposal programme on the objective of the safety case at hand. The most relevant decisions made by ONDRAF/NIRAS are:

- 1) The long term management of category B&C wastes requires a solution on the national territory.
- 2) The potential host formations for a geological repository are limited to poorly indurated argillaceous formations, with the Boom Clay as a reference host formation and Ypresian clays as an alternative.
- 3) Waste types shall be divided into groups to be emplaced in separate sections of the repository.
- 4) There are preferences for permanent shielding of the wastes and for minimisation of operations in the underground.

Engineering and scientific studies as well as safety&feasibility assessments are guided by the application of fundamental principles established by the IAEA such as passive safety, defence-in-depth (by the use of multiple safety functions), robustness, demonstrability of the safety case (by multiple evidences), best-available technology and optimization. The safety strategy culminates with the safety concept. The set of requirements derived from the strategic choices

and from the safety principles and the boundary conditions results in the derivation of a safety concept, i.e. the broad, high-level description of how the disposal system will provide safety in the long-term. The safety concept is further discussed in the next section.

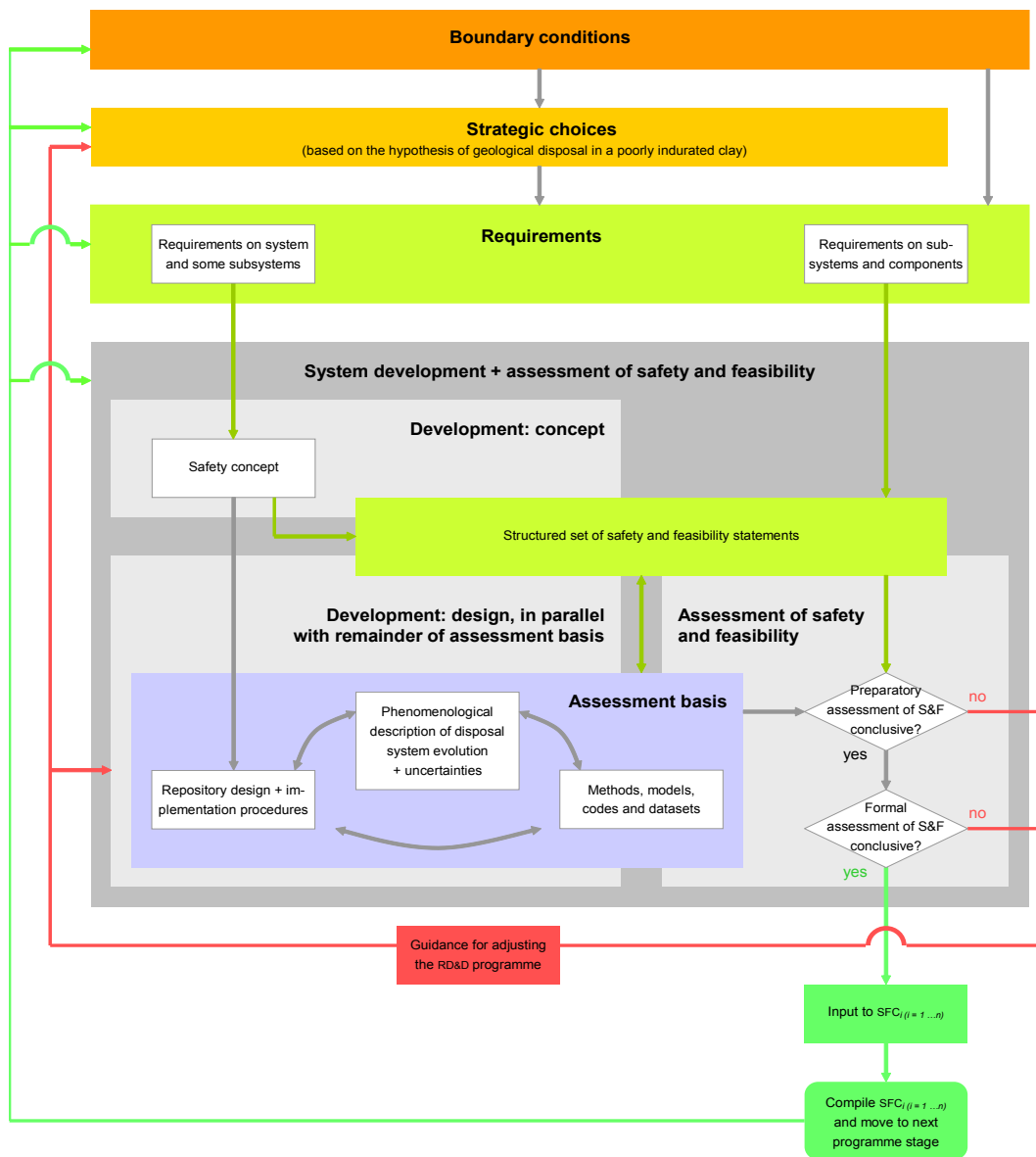


Figure 1: Overview of the safety strategy (ONDRAF/NIRAS, 2009a)

The safety concept is translated into a hierarchical structured set of so-called “safety and feasibility statements”, forming the cornerstone of the application of the safety strategy (ONDRAF/NIRAS 2009a; Depaus and Capouet, 2012). Safety and feasibility statements, and the assessment of the level of support that is available for them, provide a useful tool to steer research and development activities, to guide the application of quality assurance procedures (such as completeness checks of the assessment basis and of safety and feasibility assessments, via lists of features, events and processes), and to structure the documentation of safety and feasibility cases.

The top-level statements define the main objectives of the safety and feasibility assessment, namely demonstrating that the disposal system can provide long-term safety and that it is

feasible to implement. Lower-level statements setting out more detailed requirements of these objectives are then derived from these top-level statements in a top-down approach.

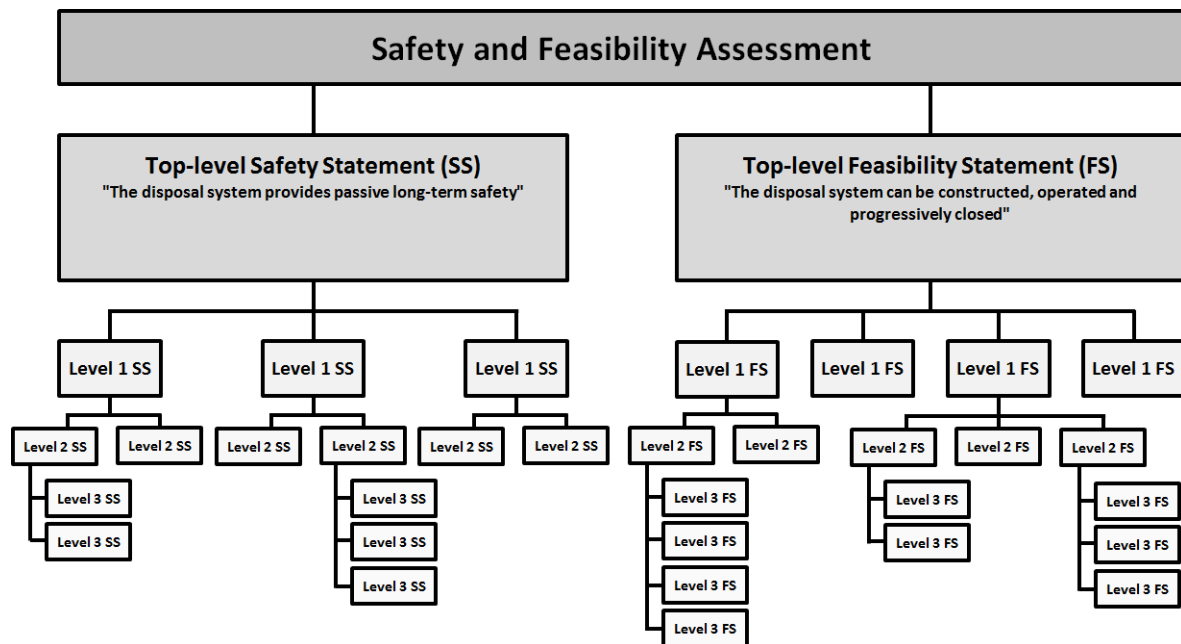


Figure 2: Schematic representation of the tree structure for the safety and feasibility statements

On the contrary, substantiation of the safety&feasibility statements with the multiple lines of evidence and their associated uncertainties generated from the RD&D programme is performed bottom-up. The assessment of the level of support given to the statements and the impact of the associated uncertainties to the higher-level statements provide an efficient and synoptic tool to steer the research and development activities and set the priorities.

With the safety concept as a basis, the development of a repository design (and, as the programme matures, the development of implementation procedures), is carried out iteratively, in parallel with the continuous development of the assessment basis, comprising the existing knowledge and understanding and the analysis tools, and with so-called “preparatory safety and feasibility assessments”. Preparatory assessments aim to assess the impact of uncertainties on long-term safety and feasibility, qualitatively and, to the extent possible, quantitatively. Together with the development of the assessment basis, preparatory assessments generate multiple lines of reasoning, arguments and analyses to support safety and feasibility statements. They also aim to identify any significant deficiencies in current knowledge and understanding and to set up the plans to address these in the research and development programme. Modifications can then be made in the programme and, should this appear necessary, in the strategic choices.

Formal assessments of the proposed disposal system are carried out provided preparatory assessments indicate good prospects that these will confirm the safety and feasibility of the repository to the extent needed for the programme stage at hand. The formal assessments should provide a finer understanding of the remaining uncertainties and their safety relevance.

1.2.2 The safety concept

The safety concept is the integrated description of the elements on which the passive long-term safety of the proposed system rests (Figure 3). This description, which is given at a level of detail

appropriate to the stage of disposal system development, includes (1), the safety functions provided by the main components of the system and its geological coverage and (2), the features of the system and its implementation providing robustness by ensuring that each of the safety functions will, in reality, be fulfilled over at least the assigned time frames, irrespective of any remaining uncertainties.

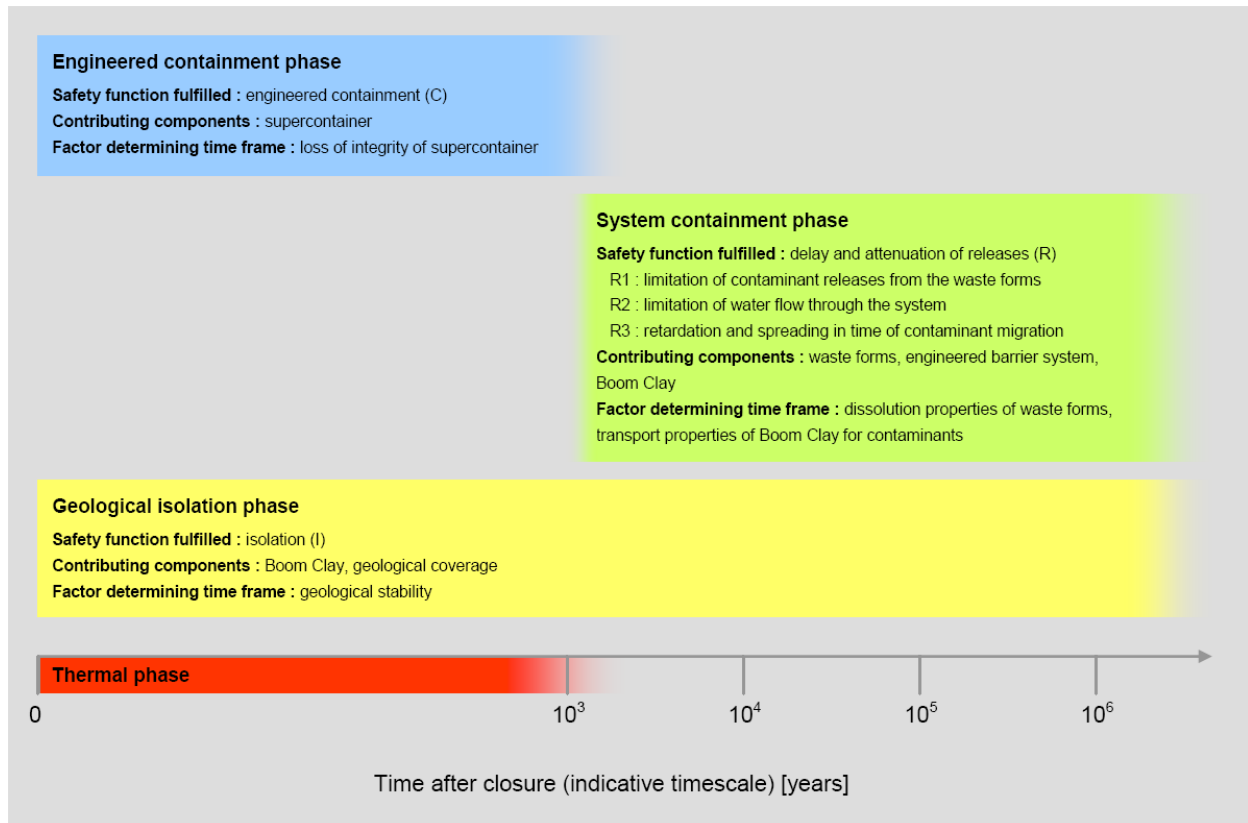


Figure 3: Safety functions provided by the main components of the disposal system for category C waste and time frames in which they are expected to operate (ONDRAF/NIRAS, 2009b).

1.2.3 The disposal system and its environment

The *disposal system* includes engineered barriers and a natural barrier provided by the host clay formation (Boom Clay as reference and Ypresian Clay as alternative). The combination of both engineered and natural barriers ensures radiological safety in short and long-term, through the fulfillment of safety functions. The disposal system is surrounded by its *environment* which consists of the geological layers surrounding the host clay formation and a biosphere. The biosphere is defined as that part of the environment that is easily accessible for man and its activities.

The primary component of the disposal system from the point of view of long-term safety is the host (poorly indurated) clay formation. In the case of the Boom Clay, overlying sedimentary formations (a.o. sandy aquifers) protect the host formation from surface processes and events, as well as from future human actions that might perturb the safety functions provided by the repository system.

Engineered barriers reduce (or mitigate the effects of) perturbations to the host formation caused by repository construction (for example, backfilling and sealing). For category C waste, they also

eliminate the need to model migration processes during the initial transient periods of the repository lifetime, of which the thermal phase is the most important one.

1.2.4 *The safety functions*

The following safety functions are identified in the Belgian programme for radioactive waste management:

- The *isolation* (I) safety function is provided by the Boom Clay and overlying formations and is expected to remain fulfilled into the far future. The repository is located at sufficient depth from the biosphere and far enough from exploitable underground resources to reduce the likelihood of inadvertent human intrusion.
- The *engineered containment* (C) safety function is specific to heat-generating waste (category C waste) and is guaranteed by the extremely low corrosion rate of the carbon steel overpack within a high-*pH* environment imposed by the OPC-based concrete buffer. Referring to the safety concept, this safety function is supposed to be fulfilled at least during the thermal phase¹, which may last a couple of thousand years in case of spent fuel disposal. By completely containing the radionuclides during the thermal phase, no radionuclide migration through the host rock will occur when the host rock has an elevated temperature. This simplifies the assessment of the migration processes and increases the robustness of the disposal system. Containment of heat-emitting radioactive waste is a requirement imposed by international regulations (IAEA, 2011) and is included in the boundary conditions of the ONDRAF/NIRAS safety strategy (ONDRAF/NIRAS, 2009a). In the reference design, containment is provided by the so-called supercontainer (see section 3.1.1)
- The *delay and attenuation of the releases* (R) safety function is provided by the complete disposal system with Boom Clay being again the main contributor. This safety function will be fulfilled into the far future, because of the stability of the physical and chemical properties of the host formation and because of the resistance to leaching of the waste form. It may be subdivided into three contributing subfunctions:
 - *limitation of contaminant releases from the waste forms* (R1)
This subfunction essentially represents the resistance to leaching of the contaminants from the waste form, which is governed by various physico-chemical processes, such as slow dissolution mechanisms and precipitation.
 - *limitation of water flow through the system* (R2)
Because of appropriate favorable features of the host clay, such as a fine porosity, a very low hydraulic conductivity and the absence of reservoirs of mobile water, and limited driving forces for water flow (notably the small hydraulic gradient over the formation), water flow through the system is negligible. Consequently, the dominant solute transport mechanism in the disposal system is diffusion.

¹ The thermal phase is defined as the time frame during which the temperature of the host formation is expected to lie above the range of temperatures within which nominal migration properties can be relied upon. See also section 4.4.1.

- *retardation and spreading in time of contaminant migration (R3)*
Processes such as diffusion, (secondary) precipitation and various sorption processes within the host formation contribute to this subfunction. As such, any contaminants released from the repository will decay or be contained virtually completely within the Boom Clay for a period of at least a few tens of thousands of years, and the many contaminants that are subject to significant geochemical retardation will be contained for even longer.

As defined in the safety concept, appropriate siting and design will ensure that the safety functions are fulfilled during the required period by providing geological stability and intrinsic robust features such as chemical buffering capacities and self-sealing.

The processes of “dispersion and dilution” that operate once the dissolved elements from the waste form leave the clay host rock and enter the surrounding aquifers are considered as a role of the environment of the repository but not as a safety function, because all efforts made to maximize or optimize them would lead to a “disperse and dilute” strategy, instead of the chosen strategy to “concentrate and confine” the waste. A more detailed discussion on safety functions can be found in ONDRAF/NIRAS (2007a), De Preter *et al* (2006) and Depaus and Capouet (2012).

The processes and components contributing to the safety functions are listed in Table 1.

Table 1: *Components and processes contributing to the safety functions.*

Safety (sub)function	Components/processes
Reduction of likelihood and consequences of human intrusion (I)	Host formation and overlying formations by selection of appropriate depth
Engineered containment (C)	Carbon steel overpack in high-pH environment (supercontainer concept) ensuring passive corrosion
Limitation of releases (R1)	Leaching resistance and stability of waste forms/matrices Near field solubility
Limitation of water flow (R2)	Low-permeable host formation No enhanced transport through engineered barriers (use of seals) Limited driving forces for flow (especially hydraulic gradients), both natural or induced
Retard migration (R3)	Sorption processes Far field solubility

The availability of the safety functions at the time at which they should be effective forms the basis for the definition of the reference scenario and reference case (NEA, 2011; see Chapters 4 and 5).

1.3 Methodology for safety assessments in the SFC1 framework

1.3.1 Overview

An overview of the safety assessment methodology is given in Figure 4 and discussed further in the safety assessment methodology document (ONDRAF/NIRAS, 2009c). Safety assessment requires a detailed knowledge base and adequate analysis tools, collectively termed the assessment basis. The assessment basis includes:

- The description of the design of the proposed disposal system and, depending on the stage of planning and development, implementation procedures: this aspect of the assessment basis falls within the scope of the “technology pole” of the RD&D programme;
- The empirical and theoretical scientific knowledge and understanding that are relevant to the assessment of the safety and feasibility of the disposal system under consideration, including relevant process models and computer codes, a description of the expected phenomenological evolution of the system, and the scientific knowledge and understanding underlying this description, including associated uncertainties: this aspect of the assessment basis falls within the scope of the “phenomenology pole” of the RD&D programme;
- The various methods, models, computer codes and datasets for assessing safety and feasibility, including the safety assessment methodology and the feasibility assessment methodology: this is termed the “toolbox” by ONDRAF/NIRAS.

Safety assessments in the SFC1 framework consist of the preparatory and the formal phase. Preparatory safety assessments aim to identify potentially safety-relevant uncertainties, to provide partial, quantitative assessments of their impact on system performance and safety. This phase is characterized by intense interactions between the tree poles: Safety, Phenomenology and Technology. The constant and iterative interaction between these three poles leads to construct and refine the assessment basis based on the safety concept and in agreement with the safety strategy.

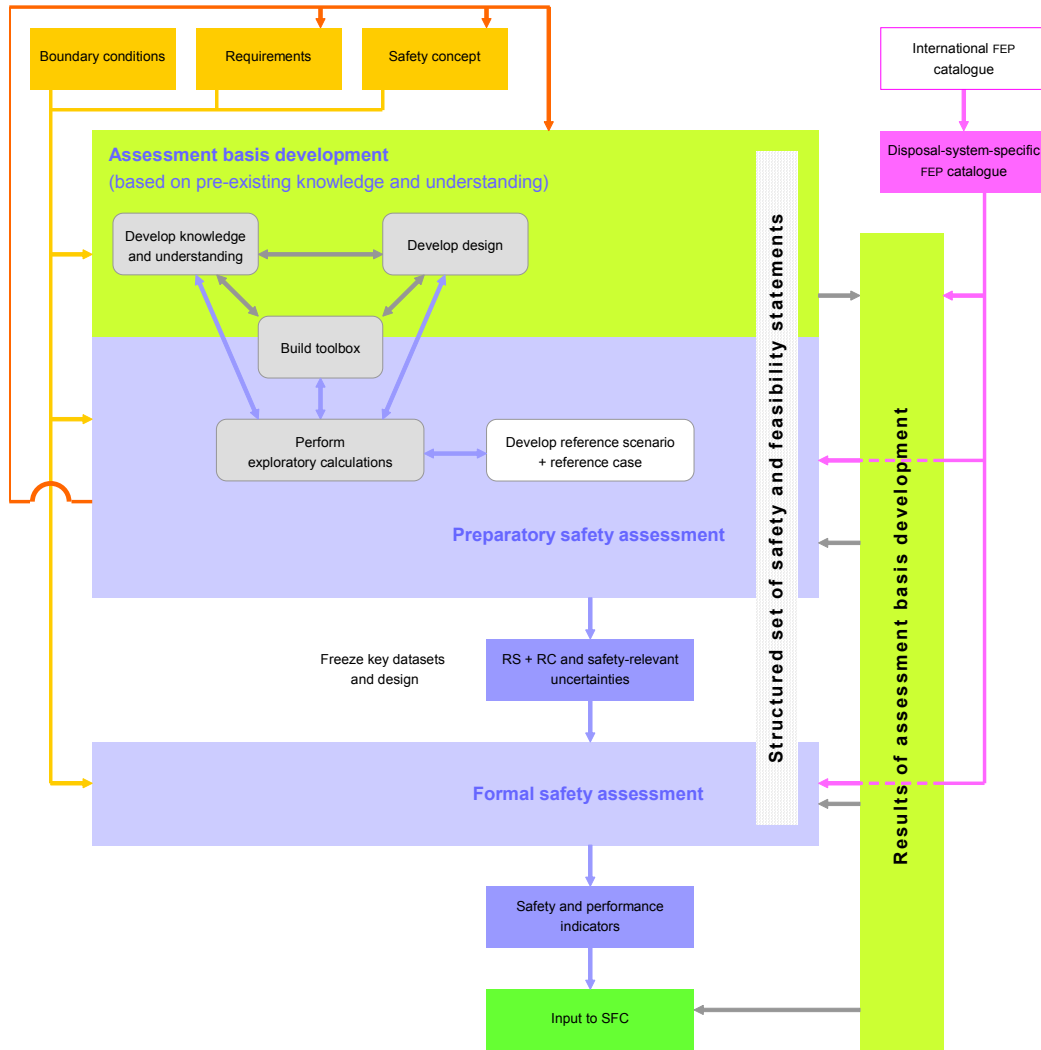


Figure 4: Overview of the safety assessment methodology (ONDRAF/NIRAS, 2009c)

Preparatory safety assessments are conducted simultaneously with works on repository development and system understanding. They take the form of exploratory calculations or safety calculations. The first calculations aim to study the behaviour and/or the sensitivity of key process(es) or feature(s) potentially relevant to the long-term safety of the disposal system. The latter type of calculations aims the modeling of the migration of the contaminants throughout the disposal system to the biosphere. They give a quantitative assessment of the performance and safety of the system with the use of safety and performance indicators. These calculations entail sustained, structured interactions between safety assessors and experts in phenomenology and technology. Preparatory assessments also aim to identify any significant deficiencies in current knowledge and understanding and set up the plans to address these in the RD&D programme, thus providing feedback to assessment basis development. Through these preparatory assessments of various natures, the safety analysts gain stepwise a confirmation that the disposal system will evolve as defined in the safety concept, fulfilling each safety function as required. The evolution drawn by the safety concept is called the reference scenario.

One tool used to challenge the progress of the R&D in term of its impact on the long-term safety is the working version of the reference case. The reference case is a specific realisation of the reference scenario associated to a conservative or more realistic, well justified set of parameter

values and choices. This reference case, being based among the most conservative –and therefore most defensible– hypothesis, can be considered as a yardstick to guide the RD&D programme. Several working versions of the reference case are iterated before a final version associated to a comprehensive set of uncertainties is completed. During this preparatory phase the results of the working versions of the reference case provide a snapshot of the level of safety that the current results of the RD&D programme can support. These working versions give insights on the impact of various uncertainties and guidance to future RD&D and expert discussions. Uncertainties are here to be understood in its broader sense and encompass all perturbing FEPs of low expectation (e.g geologic events), uncertainties bound to expected processes, on the level of models and parameters. Challenging the uncertainties against the safety functions is carried out through the safety branch of the safety statements (Depaus and Capouet, 2012).

Formal safety assessments aim to show in a formal, quantitative way why the disposal system under consideration despite the existence of remaining uncertainties can be judged to be safe with respect to all relevant regulatory and stakeholder requirements of the programme objective at hand. Formal safety assessments are quantitative and as exhaustive as possible, and are conducted only every few years, shortly before the planned compilation of a safety and feasibility case. They aim to illustrate by a selection of calculation cases and indicators, the robustness of the system towards low probability scenarios short-cutting one or several safety functions (altered scenarios), or by describing alternative evolutions which do not affect the safety concept of the system (alternative cases within the reference scenario). The different sets of calculations illustrated in the safety case will also aim at quantifying the safety margins between the reference case generally based on conservative hypothesis and other more realistic realisations. The formal safety assessments are strongly dedicated to illustrate how the system fulfils the regulatory and stakeholder requirements and to highlight and prioritize the main open issues left to be treated in the next programme stage. Formal assessment phase start after all key datasets are frozen. Interactions between the three poles remain however important to ensure that the phenomenological and technological uncertainties are well understood and correctly abstracted in the scenarios and calculation cases.

Ultimately safety assessments will show that the uncertainties associated to the assessment basis sorted out in the phenomenological branch of the safety statements do not call into question the the safety functions related statements.

1.3.2 Methodology for the treatment of parameter uncertainty

The management of parameter uncertainties during the preparatory phase is carried out step-wise according to the spatial and temporal dimension. The applicability of the data are considered successively from the following three angles: upscaling, evolving conditions and transferability. This progressive treatment favours traceability and understanding of the origin of parameter uncertainties. These three steps are defined as:

- **Upscaling:** refers to the applicability of the phenomenological data collected at the scale of the laboratory over relatively short intervals of space and time to a larger spatial scale of interest in the safety assessment.
- **Evolving conditions:** refers to the impact on the phenomenological data obtained today of phenomena occurring over time that may affect the disposal system, such as phenomena occurring within the disposal system or induced by external events.

- **Transferability:** addresses typically the transfer of parameter values from boreholes to the whole zone considered for disposal (e.g. hydraulic parameters). In other words, this step includes horizontal variability of parameters within the disposal zone.

Furthermore, when the determination of a probability density function is not possible because of a lack of sufficient data or converging arguments, the uncertainty of the safety relevant parameters is expressed by two intervals (Depaus and Capouet, 2011):

- The **expert range (ER)** is the range within which an expert expects the parameter value to lie. This range is also referred to as the realistic or likely range.
- The **source range (SR)** is the range outside which the experts do not expect the parameter value to lie. This range is also referred to as the support range.

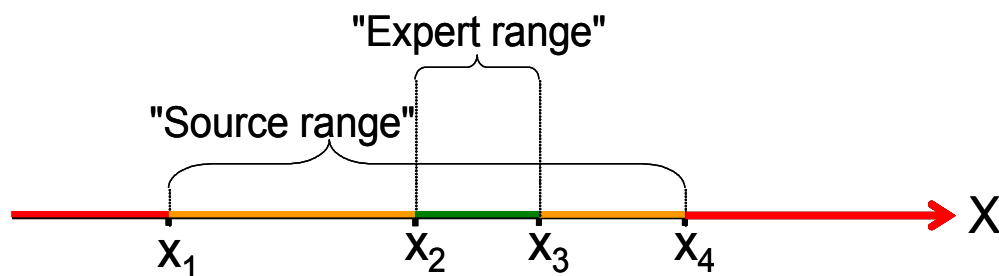


Figure 5: Representation of source and expert ranges. $[x_2, x_3]$ = range within which the value of X should lie, to the best of the experts knowledge i.e. “(fully) realistic values”; $\setminus]x_1, x_4[$ = range of values that should be ruled out for X , to the best of the experts knowledge, i.e. “unrealistic” (or “unsupported”) values; $]x_1, x_2[\cup]x_3, x_4[$ = range of values that experts cannot entirely rule out for X , but which would be somewhat surprising, i.e. somewhat less “realistic”.

1.4 Scope of this document

This document presents the state of the art description of the reference scenario and the reference case on the basis of the assessment basis developed so far in 2011 in the framework of the preparatory safety assessment phase. It provides a synthesis of the expected phenomenological evolution (Chapter 4) of the system and describes how this information supports the reference scenario. Moreover, it describes how the safety relevant processes are conceptualised or abstracted in the third working version of the reference case (Chapter 5). Chapter 6 provides more information on the iterative process that has been followed to develop the different versions of the reference case up to the current one.

Note that the current reference case focuses mainly on the upscaled uncertainties. Some uncertainties pertaining to “evolving conditions” (e.g. climate evolution) and “transferability” (e.g. variation of chemical conditions, influence of depth) have not yet been fully treated in this preparatory phase and their radiological impacts are not discussed in this document. These uncertainties may give rise to alternative cases or a specific case from an altered scenario. The working reference case focuses on the uncertainties bound to a repository constructed at depth in Mol where the physico-chemical conditions of the far field remain unchanged in the long-term. The reference case, being based on conservative hypotheses, makes use of the pessimistic bounds of the expert ranges for the safety parameters for calculating the radiological impact of a repository for category B and C waste in Boom Clay.

2 Radioactive waste specifications

This chapter first presents the classification used in Belgium for radioactive waste (section 2.1). Then, estimations of waste volumes and radionuclide inventories per waste type are provided in sections 2.2 and 2.3, respectively. Section 2.4 describes the characteristics of the different waste packages after conditioning.

2.1 Belgian waste categories

For long-term management (*i.e.* disposal) of radioactive waste, ONDRAF/NIRAS has adopted a method for classifying conditioned radioactive waste based on three general (A, B and C) and one special (R) categories. This classification method is compatible with those of the International Atomic Energy Agency (IAEA, 2009) and the European Union (EC, 1999). It categorises radioactive waste according to its activity level and life span (see Figure 5). The half-life of radionuclides present in the waste determines the long-term management.

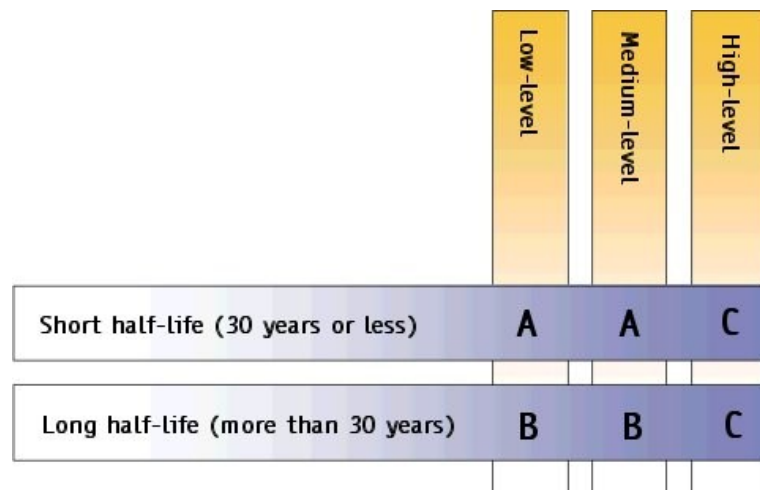


Figure 6: ONDRAF/NIRAS' waste classification for long-term waste management.

Category A waste is conditioned waste containing radionuclides of a sufficiently low activity level and with a sufficiently short half-life to allow surface disposal. It includes low or intermediate-level and short-lived waste, *i.e.* waste containing radionuclides for which the majority have a half-life of less than or equal to 30 years. This waste may contain traces of long-lived alpha emitters. This category of waste should be isolated from man and the environment for at least 300 years, which is the time necessary for their activity level to decrease by a factor of 1 000.

Category B waste consists of conditioned low and intermediate-level waste contaminated by long-lived radionuclides, in particular alpha emitters, in quantities that are too large for this waste to be classified as category A, but which emit too little heat to belong to category C. This waste may also contain varying quantities of beta and gamma emitters.

Category C waste includes all conditioned high-level waste containing significant amounts of beta and gamma emitters with a short half-life and large quantities of long-lived radionuclides, in particular alpha emitters. Because of the high activity level, most of the waste in this category emits considerable amounts of heat.

Category B and C waste, which contains significant quantities of radionuclides with a half-life longer than 30 years, should be isolated from man and the environment for many thousands of

years. There is a world-wide scientific and technical consensus today that geological disposal is the safest and most sustainable management option to deal with this waste (NEA, 2008; EC, 2011) and that this solution complies with basic ethical principles (NEA, 1995). In principle, all foreseeable category B&C waste fluxes that are expected to occur in Belgium will be evaluated in SFC1. However, in the preparatory safety assessments, only a limited but representative set of waste types are treated.

In practice, waste acceptance criteria determine which waste is acceptable for surface disposal. These criteria are maximum activity concentration and total activity. Site-specific performance assessment calculations (capacity calculations) are necessary to evaluate which wastes can be accepted in the considered surface disposal facility. On the basis of these types of evaluations, it is possible that some waste types currently considered as category A waste would be reclassified as category B waste. Similarly, the condition that the Boom Clay may not be heated above 25°C (corresponding to a temperature increase of 9°C at the reference site) for category B waste will determine the waste classification. Therefore, the distinction between category B and C waste not only depends on the volumetric heat production of the waste, but also on the waste disposal density and the host rock properties in terms of heat dissipation. Detailed heat transport calculations are performed in support of the waste classification process.

Category R consists of waste contaminated by radium. Large amounts of this waste are currently stored on the UMICORE site at Olen.

2.2 Spent fuel management scenarios and waste volumes

2.2.1 Waste volumes due to electricity production

The present Belgian nuclear power park consists of seven nuclear reactors: four at Doel and three at Tihange. The total installed nuclear power is 5935 MW(e) or 5.9 GW(e) (see Table 2). For an operational period of 40 years, the total amount of nuclear fuel that will be irradiated in the Belgian reactors is estimated to be 5339 tHM. The category C waste inventories that will be considered in the present report thus correspond to the nuclear fuel that will be irradiated in the existing Belgian nuclear power plants over an operational period of 40 years.

Table 2: Capacity and start of electricity production of the Belgian nuclear power plants.

Reactor	Capacity MW(e)	Start
Doel 1	433	1975
Doel 2	433	1975
Doel 3	1006	1982
Doel 4	1039	1985
Tihange 1	962	1975
Tihange 2	1008	1983
Tihange 3	1054	1985
Total	5935	

Before 1993, when the reprocessing moratorium came into force in Belgium, 630 tHM spent uranium oxide fuel have been sent to La Hague for reprocessing. The recuperated Pu has been recycled as 66 tHM MOX (mixed oxide) fuel in two reactors (Doel 3 and Tihange 2). The waste

arising from the reprocessing of those 630 tHM spent fuel are 390 vitrified high-level waste canisters (category C waste) and 534 canisters containing compacted hulls and structural elements (category B waste).

Thus, in the first spent fuel management scenario, if the reprocessing moratorium and the nuclear phase out are maintained in Belgium, the electricity production in the seven Belgian nuclear reactors will lead to the generation of the following amounts of category B&C waste:

- cat. B waste: 534 canisters (150 l) with compacted hulls and structural elements;
- cat. C waste: 390 canisters (150 l) with vitrified high-level waste;
- cat. C waste: 4643 tHM uranium oxide (UOX) spent fuel;
- cat. C waste: 66 tHM spent MOX fuel.

The number and lengths of the spent fuel assemblies that are expected to arise from this scenario are given in Table 3.

Table 3: Number of fuel assemblies expected to arise from the electricity production in Belgium for a 40-year operation of the existing power plants.

Reactors	Fuel type	Assembly length (feet)	Burn-up (GWd/tHM)	Number
Doel 1/2	UOX	8	36-55	1750
Doel 3 / Tihange 1/2	UOX	12	36-62	4940
Doel 4 / Tihange 3	UOX	14	36-62	3537
Doel 3 / Tihange 2	MOX	12	45-50	144

A second spent fuel management scenario will also be considered in SFC1, in which it is assumed that all the UOX spent fuel will be reprocessed. On the other hand, as MOX spent fuel is not reprocessed in the reprocessing plants at La Hague (France) or Sellafield (UK), it is assumed that the MOX spent fuel will not be reprocessed. Also in this scenario, it can be expected that the vitrified high-level waste and the compacted hulls and technological waste will return to Belgium. On the other hand, it is assumed that the recuperated Pu, which is not considered as waste but as fissile material, will remain in the country where the spent fuel is reprocessed. This variant spent fuel management scenario would lead to the generation of the following amounts of category B&C waste:

- cat. B waste: 4294 canisters (150 l) with compacted hulls and technological waste;
- cat. C waste: 3220 canisters (150 l) with vitrified high-level waste;
- cat. C waste: 66 tHM spent MOX fuel.

In the first series of calculations of the preparatory safety assessments, notably the calculations for working versions 1 and 2 of the reference case, the MOX spent fuels and the compacted hulls and technological waste were not taken into account. In those calculations, only two types of high-level waste inventories were considered:

- 'Spent Fuel': 4643 tHM UOX spent fuel;
- 'VHLW': 3220 canisters (150 l) with vitrified high-level waste.

The preparatory safety assessments calculations for version 3 (*i.e.* the version presented in this report) have been made for all major waste streams: UOX and MOX spent fuel, vitrified high-level waste and compacted hulls and technological waste. In the formal safety assessments of the SFC1, evaluations of the radiological impact of the disposal of all the B&C waste types corresponding to each spent fuel management scenario will be made.

2.2.2 Historical waste volumes

The pilot scale reprocessing plant Eurochemic at Dessel was operated by an international consortium of OECD countries between 1966 and 1974. In total about 180 tonnes of natural and low-enriched uranium spent fuels from power reactors and about 30 tonnes of high-enriched uranium spent fuels from research reactors were reprocessed. The most active waste types that arose from these reprocessing activities are about 2200 canisters containing vitrified waste that were produced in the PAMELA vitrification plant between 1985 and 1991 (HAGALP1 and HAGALP2), 115 canisters cemented waste (HAGALP3), and about 13550 drums containing intermediate-level waste conditioned in a bitumen matrix (MAGALE); this last waste type is known as Eurobitum waste.

Because of its very specific near field behaviour, the radiological consequence analysis of the disposal of Eurobitum waste in Boom Clay is treated in a separate report (Weetjens, to be published). These calculations are based on the present conceptual model description of the reference case (version 3). The last iteration of safety assessment calculations for the PAMELA waste types was done in 2008 (Raeymaekers *et al.*, 2008), and was not updated in the frame of the preparatory safety assessment.

2.3 Radionuclide inventories

The inventory for both spent fuel and vitrified high-level waste is provided by ONDRAF/NIRAS (“SFC1-data-110211-v1.13.xls”) for a reference time of 10 years after unloading the spent fuel from the reactor. Based on these data, the respective inventory data are calculated taking into account a total cooling time of 60 years for category C waste.

2.3.1 UOX spent fuel

Different types of PWR nuclear reactors have been built in Belgium. As a consequence, fuel assemblies with different length are used (8ft, 12ft and 14ft; cf. Table 3). The burn-up in the Belgian reactors has been increased progressively from 33 to 62 GWd/tHM. Low burn-up fuels from the Doel 1, Doel 2 and Tihange 1 reactors have been reprocessed at La Hague. The inventory of the different types of UOX assemblies are represented by an "average" UOX assembly that strongly resembles a 12ft assembly². Averaging the source term for assessing radiological consequences can be justified, because at the level of the Boom Clay – aquifer interface, the concentrations will be spread over the whole repository footprint, and a water well will draw water from a large volume. The radionuclide inventory provided by ONDRAF/NIRAS corresponds to an average burn up of 47.3 GWd/tHM (based on the amount of fission products, which increase linearly with burn-up) and an initial enrichment of 4.05% ²³⁵U (see Table 4).

² The total gallery length necessary to reconstitute the total inventory from the “averaged” reference spent fuel assembly is 14.06 km.

Table 4: Spent fuel radionuclide inventory of an "average" UOX assembly after 10 years of cooling. Only the PA-relevant fission and activation products and actinides are given.

Nuclide	Inventory/assembly (Bq/ass)	Total inventory (Bq)	Nuclide	Inventory/assembly (Bq/ass)	Total inventory (Bq)
C14	5.68E+10	5.81E+14	Ra226	7.34E+03	7.51E+07
Cl36	3.25E+09	3.32E+13	Th229	8.37E+03	8.56E+07
Ca41	1.50E+09	1.53E+13	Th230	2.44E+06	2.50E+10
Ni59	3.75E+10	3.84E+14	Th232	3.71E+00	3.79E+04
Se79	9.89E+08	1.01E+13	Pa231	4.78E+05	4.89E+09
Zr93	4.68E+10	4.79E+14	U233	6.49E+05	6.64E+09
Nb94	4.60E+10 (*)	4.70E+14	U234	5.31E+10	5.43E+14
Tc99	2.91E+11	2.97E+15	U235	5.66E+08	5.79E+12
Pd107	3.05E+09	3.11E+13	U236	8.92E+09	9.12E+13
Sn126	1.98E+10	2.03E+14	U238	5.24E+09	5.36E+13
I129	7.47E+08	7.64E+12	Np237	2.84E+10	2.91E+14
Cs135	1.14E+10	1.16E+14	Pu244	2.79E+04	2.85E+08
			Cm248	1.39E+05	1.42E+09

(*) a higher Nb-94 inventory has been considered in the calculations for Versions 1 and 2, because it was assumed that all the claddings were made of the M5 alloy (see section 2.4.4), whereas now it is assumed that 20% is made of M5 and the other 80% of Zircaloy-4)

The spent fuel waste inventory is based on a scenario corresponding to a lifetime of 40 years for current nuclear power reactors with a capacity of 5.9 GW(e). Only the radionuclides relevant for evaluation of long-term radiological safety are given in the inventory tables. For a detailed explanation on the selection of radionuclides and treatment of actinide chains, see the Annex.

2.3.2 MOX spent fuel

The 66 tHM MOX fuel assemblies have been irradiated in the Doel 3 and Tihange 2 reactors to a burn-up of 50 GWd/tHM; the initial enrichment was about 7.7% Pu. The radionuclide inventory per assembly is given in Table 5.

Table 5: Spent fuel radionuclide inventory of a MOX assembly (BU: 50GWd/tHM) after 10 years of cooling. Only the PA-relevant fission and activation products and actinides are given.

Nuclide	Inventory/assembly (Bq/ass)	Total inventory (Bq)	Nuclide	Inventory/assembly (Bq/ass)	Total inventory (Bq)
C14	3.39E+10	4.88E+12	Ra226	3.16E+03	4.56E+05
Cl36	1.78E+09	2.57E+11	Th229	2.70E+03	3.89E+05
Ca41	7.73E+08	1.11E+11	Th230	1.34E+06	1.93E+08
Ni59	3.17E+10	4.57E+12	Th232	1.64E-01	2.36E+01
Se79	8.59E+08	1.24E+11	Pa231	4.20E+04	6.05E+06
Zr93	3.47E+10	5.00E+12	U233	1.69E+05	2.43E+07
Nb94	6.44E+09	9.27E+11	U234	2.33E+11	3.35E+13
Tc99	3.09E+11	4.45E+13	U235	8.25E+08	1.19E+11
Pd107	6.76E+09	9.74E+11	U236	1.92E+10	2.77E+12
Sn126	2.70E+10	3.90E+12	U238	5.09E+09	7.33E+11
I129	1.01E+09	1.46E+11	Np237	1.22E+11	1.75E+13
Cs135	1.65E+10	2.38E+12	Pu244	3.09E+05	4.45E+07
			Cm248	3.40E+06	4.89E+08

2.3.3 *Vitrified high-level waste (CSD-V canisters)*

The radionuclide inventory of the 390 existing canisters is estimated on the basis of information provided by Areva, and is provided in the O/N data spreadsheet "SFC1-data-110211-v1.13.xls". This datasheet also provides inventory estimates for the 2830 canisters that will arise if all the UOX spent fuels are reprocessed. These estimates are made on the basis of the radionuclide inventory of the spent fuel as given above, and by assuming that one canister will contain the waste arising from 1.62 tHM UOX spent fuel, as it is the case for the existing canisters which have arisen from the reprocessing of low burn-up (mainly 33 GW/tHM) spent fuels. The radionuclide inventory given in Table 6 represents a weighted average of the already produced and the foreseen canisters in case of full reprocessing.

Table 6: Average inventory of a CSD-V canister in the assumption of full reprocessing (reference time: EOL³ + 10y). Only the PA-relevant fission and activation products and actinides are given.

Nuclide	Inventory/canister (Bq/can)	Total inventory (Bq)	Nuclide	Inventory/canister (Bq/can)	Total inventory (Bq)
C14	1.46E+10	4.72E+13	Ra226	2.57E+04	8.29E+07
Cl36	1.02E+10	3.29E+13	Th229	2.82E+04	9.10E+07
Ca41	5.27E+09	1.70E+13	Th230	7.33E+06	2.36E+10
Ni59	2.16E+10	6.96E+13	Th232	1.09E+01	3.50E+04
Se79	3.47E+09	1.12E+13	Pa231	1.66E+06	5.35E+09
Zr93	1.50E+11	4.84E+14	U233	2.80E+05	9.01E+08
Nb94	1.74E+07	5.59E+10	U234	4.84E+08	1.56E+12
Tc99	1.03E+12	3.32E+15	U235	3.05E+07	9.82E+10
Pd107	1.06E+10	3.42E+13	U236	2.97E+08	9.58E+11
Sn126	6.98E+10	2.25E+14	U238	1.92E+07	6.20E+10
I129	2.64E+07	8.50E+10	Np237	5.35E+10	1.72E+14
Cs135	4.04E+10	1.30E+14	Pu244	9.28E+01	2.99E+05
			Cm248	4.50E+05	1.45E+09

2.3.4 *Compacted waste (CSD-C canisters)*

At the reprocessing plant the fuel assemblies are cut into small pieces and the cladding and structural elements are separated from the fuel pellets. The cladding and structural elements are put into compaction cans, which are then compacted to reduce their volume. Maximum 8 compacted cans are then placed in a standard waste canister, which is very similar to the canisters containing the vitrified high-level waste (see Figure 7). The "future" canisters may also contain some technological waste; this is waste that arises at the reprocessing plant from the reprocessing activities.

The average inventory of a CSD-C canister for the radionuclides relevant for long-term safety is given in Table 7.

³ EOL: End of lifetime

Table 7: Average inventory of a CSD-C canister in the assumption of full reprocessing (reference time: EOL + 10y). Only the PA-relevant fission and activation products and actinides are given.

Nuclide	Inventory/canister (Bq/can)	Total inventory (Bq)	Nuclide	Inventory/canister (Bq/can)	Total inventory (Bq)
C14	4.33E+10	1.86E+14	Ra226	1.05E+02	4.49E+05
Cl36	1.08E+09	4.65E+12	Th229	1.18E+02	5.05E+05
Ca41	6.30E+07	2.70E+11	Th230	3.52E+04	1.51E+08
Ni59	8.70E+10	3.73E+14	Th232	5.10E-02	2.19E+02
Se79	3.12E+07	1.34E+11	Pa231	6.58E+03	2.83E+07
Zr93	1.23E+10	5.28E+13	U233	1.40E+04	6.02E+07
Nb94	1.05E+11	4.51E+14	U234	1.17E+09	5.04E+12
Tc99	4.29E+09	1.84E+13	U235	1.08E+07	4.62E+10
Pd107	4.19E+07	1.80E+11	U236	1.63E+08	6.98E+11
Sn126	2.73E+08	1.17E+12	U238	7.22E+07	3.10E+11
I129	1.03E+07	4.42E+10	Np237	7.73E+08	3.32E+12
Cs135	1.57E+08	6.73E+11	Pu244	7.68E+02	3.30E+06
			Cm248	1.91E+03	8.20E+06

2.4 Type and characteristics of the primary waste packages

2.4.1 UOX spent fuel

Fuel assemblies of three different lengths (8 ft, 12 ft and 14 ft) are used in the Belgian PWR reactors. For the calculations presented in the frame of the preparatory safety assessment, only one 'average' spent fuel assembly with a length of 12 ft will be considered.

Table 8: Type and amounts of UOX spent fuel assemblies expected to arise from the Belgian nuclear power park

Assembly type	Amount	Weight (tHM/assembly)
8ft	1750	265
12ft	4940	459
14ft	3536	540
Average(12.007ft)	10226	454

The initial characteristics of the 12 ft fuel assembly are:

- initial mass of heavy metal: 459.4 kgHM
- total mass: 676.9 kg
- length: 4.058 m
- side length: 214×214 mm
- lattice: 17×17

Each spent fuel assembly is assumed to be packed in a 12 mm thick stainless steel assembly box (primary package). The assembly boxes may potentially be filled with sand, which will be rather Ca-based than Si-based. The (chemical) effects of sand on spent fuel dissolution behaviour are however not considered in the reference case.

2.4.2 *MOX spent fuel*

In total, 144 MOX fuel assemblies currently exist and are irradiated in the Belgian PWR reactors Doel 3 and Tihange 2.

The initial characteristics of the 12 ft fuel assembly are:

- initial mass of heavy metal: 456.7 kgHM
- total mass: 662.3 kg
- length: 4.058 m
- side length: 214×214 mm
- lattice: 17×17

The MOX spent fuel assembly is also assumed to be packed in a 12 mm thick stainless steel assembly box.

2.4.3 *Vitrified HLW (CSD-V canister)*

The liquid waste stream from reprocessing activities contains the fission and activation products and some actinide losses. This waste stream is vitrified by mixing with SON68 glass frit and poured into AREVA universal stainless steel canisters (CSD-V).

Two types of vitrified high-level waste are considered:

- 390 existing canisters that have arisen from the reprocessing of 630 tHM low burn-up fuels;
- 2830 canisters that will arise if all the remaining spent uranium oxide fuels are reprocessed in the future.

The main characteristics of a vitrified high-level waste canister are:

- length: 1.34 m
- external diameter: 430 mm
- wall thickness: 5 mm
- external volume: 175 l
- internal volume: 170 l
- glass content: 150 l
- mass empty canister: 80 kg
- mass vitrified waste: 412 kg

2.4.4 *Compacted waste (CSD-C canister)*

Currently 432 CSD-C canisters exist resulting from former reprocessing contracts with AREVA for recycling of spent fuel from Doel 1, Doel 2 and Tihange 1 (Boulanger, 2011a). In case a full reprocessing scenario is considered, a total of 4294 CSD-C canisters would emerge. Compacted waste consists mainly of hulls, endpieces, springs and grids of the reprocessed spent fuel assemblies and of some technological waste from the reprocessing plant. The main materials present in this waste are zircaloy (standard “Zry4”, and since 2000 the alloys “ZIRLO” and its no-tin variant “M5”) from the hulls, inconel from grids and springs and various stainless steel alloys. This waste is loaded into coated steel compaction cans (with a height of 80.2 cm and a diameter of 38.2 m, see Figure 7) and are then compacted under 200 MPa pressure. Typically 7

or 8 of these compacted discs are loaded into a stainless steel CSD-C canister. These canisters have an outer volume of about 180 ℓ and are very similar to the CSD-V canisters.

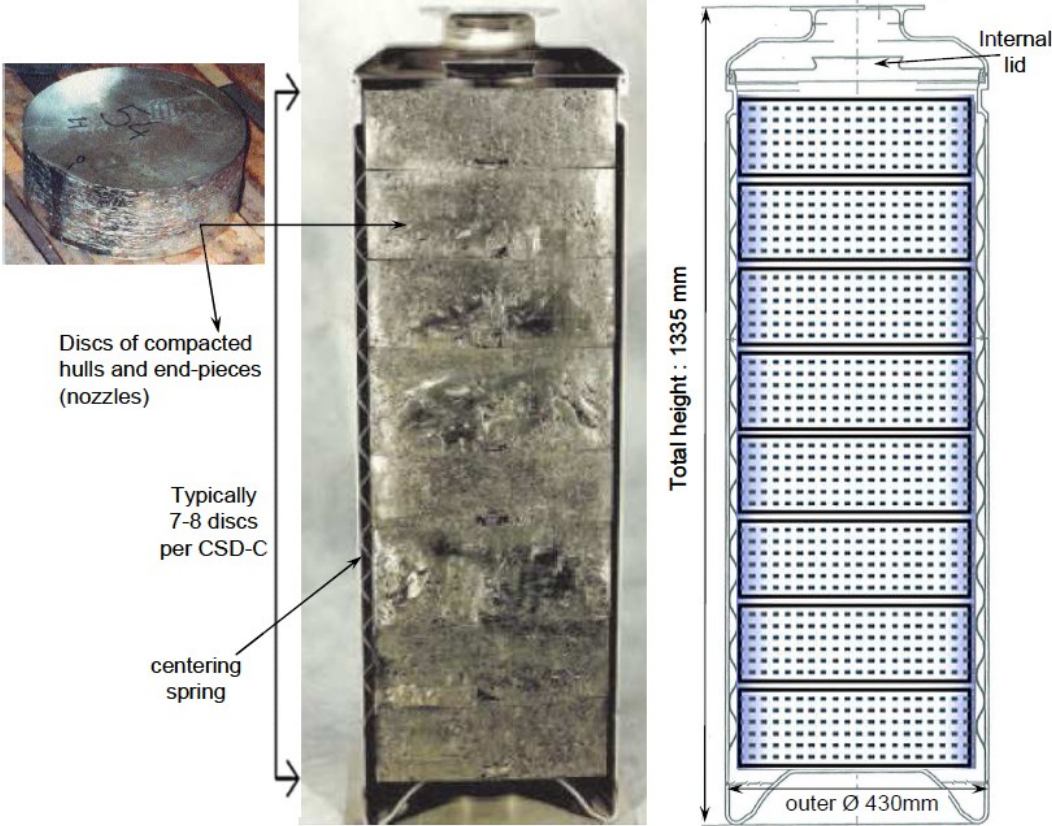


Figure 7: The CSD-C canister containing compacted hulls and end-pieces.

3 Host formation and reference repository design for Category B&C waste

The safety concept, together with the strategic choices mentioned in paragraph 1.2.3 and other boundary conditions, is the basis for developing the repository design. In the current reference repository design, the planned B&C disposal facility will be excavated at a depth of about 240 metres at the midplane of the Boom Clay layer at the reference site of Mol-Dessel. The waste will be emplaced in a set of horizontal disposal galleries, lined with concrete wedge blocks. The repository will consist of three separate sections for category C waste, historical category B waste and category B waste from reprocessing and from the operation and decommissioning of nuclear power plants and other nuclear facilities.

Important strategic choices set out by ONDRAF/NIRAS (2009a) for design development are:

- for heat-generating waste, the engineered barriers shall be designed to provide complete containment of the waste at least through the thermal phase;
- waste types shall be divided into groups to be emplaced in separate sections of the repository;
- permanent shielding of the waste is preferred and underground operations are minimised;
- materials and implementation procedures are preferred for which broad experience and knowledge already exist.

These constraining conditions have culminated into the supercontainer design for disposal of category C waste (spent UOX and MOX fuel, and vitrified high-level waste). In the supercontainer concept, the engineered barriers consist primarily of the carbon steel overpack surrounded by an OPC (Ordinary Portland Cement) concrete environment. Other auxiliary repository components, such as the backfill and gallery lining, are also based on cementitious materials. This design is expected to guarantee complete containment of the waste for several thousands of years.

Also for category B waste, concrete is heavily relied upon because of its good shielding and sorption properties, well-known behaviour (for conventional engineering applications), ease of control, availability and affordability. The category B waste will be packed in reinforced concrete containers called monoliths (similar to the containers that will be used for surface disposal of category A waste).

3.1 Engineered barrier design

3.1.1 The supercontainer

The principal component of the engineered barrier system (EBS) for vitrified high-level waste and spent fuel is the so called BSC-1 supercontainer (GSL, 2005). This design is based on the Contained Environment Concept (Wickham, 2006; ONDRAF/NIRAS, 2004) and was selected by ONDRAF/NIRAS through a multi-criteria analysis. The supercontainer comprises a carbon steel overpack and a Portland cement concrete buffer with or without an outer stainless steel envelope (Figures 8 and 9). The phenomenological description of the repository evolution does not take into account the presence of the envelope. In other words, the supercontainer design without the envelope is considered the reference engineered barrier design.

Table 9 shows the dimensions of the supercontainer and disposal gallery for UOX spent fuel and vitrified HLW.

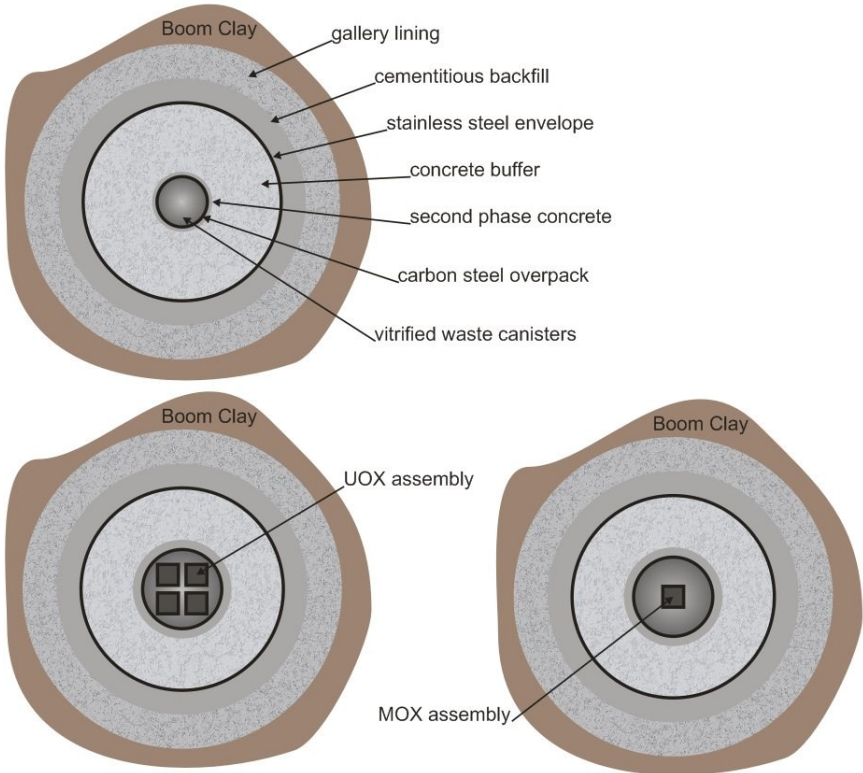


Figure 8 : Cross-section of the supercontainer concept for three high-level waste types: vitrified HLW, UOX and MOX spent fuels.

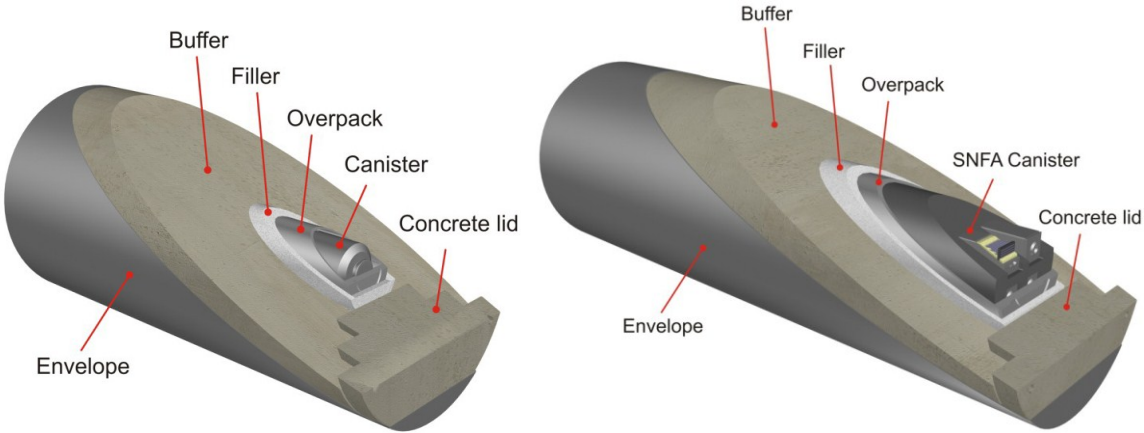


Figure 9: 3D representation of a supercontainer containing 2 canisters of vitrified HLW (left), and a supercontainer containing 4 UOX spent fuel assemblies (right).

Table 9: Dimensions (in m) of the supercontainer and disposal gallery for UOX spent fuel (12 ft assemblies) and vitrified HLW. (reference "SFC1-data-100505.xls" based on O/N-2009-0146-B&C Concept ANN4).

	UOX spent fuel (SC_SF12)	Vitrified HLW
Overpack		
• Outer radius	0.49	0.26
Buffer		
• Outer radius	1.08	1.01
• Outer length	5.50	4.07
Number of fuel assemblies/canisters per supercontainer		
	4	2
Disposal gallery		
• Inner radius	1.5	1.5
• Outer radius	1.8	1.8
• Distance between two galleries	120	50

3.1.2 The monolith

The disposal packaging system for category B waste consists of a concrete monolith. Different geometries are considered depending on the waste type. In case of compacted waste, the monolith is of type MO_180L, in which 8 CSD-C canisters can be placed (see Figure 10). The characteristics of this monolith type are provided in Table 10.

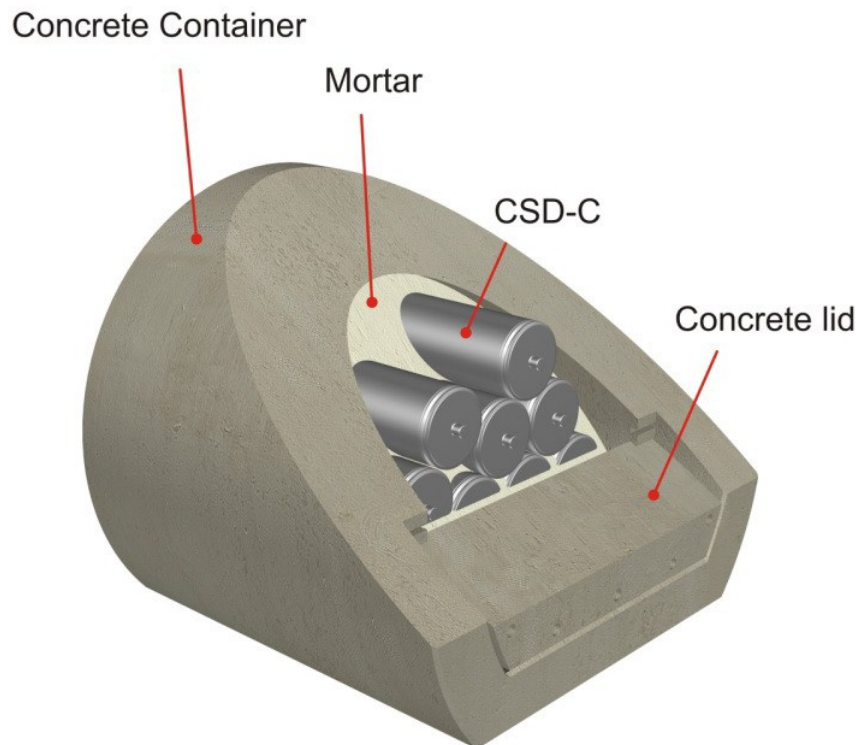


Figure 10: The monolith MO_180L for packaging the CSD-C canisters.

Table 10: Dimensions of the monolith for compacted waste.

Monolith Type	Outer length (mm)	Outer diameter (mm)	Base width (mm)	Radial thickness (mm)	Axial thickness (mm)	Mass (kg)
MO_180L	2585	2800	2120	520	560	36500

3.2 Repository design

The envisaged repository consists of a series of rectilinear galleries, in which the waste will be disposed, situated around the midplane of the Boom Clay formation. This corresponds to a depth of about 230 to 240 m at the reference site. Access to the disposal galleries is provided via the centrally located access gallery, to which all disposal galleries are linked. This access gallery will follow the natural inclination of the Boom Clay (about 1%) and is therefore oriented according to the northwest – southeast axis. In turn, the access gallery is connected to the surface via at least two shafts (ONDRAF/NIRAS, 2007b). A sketch of the different components in the disposal system is shown in Figure 11.

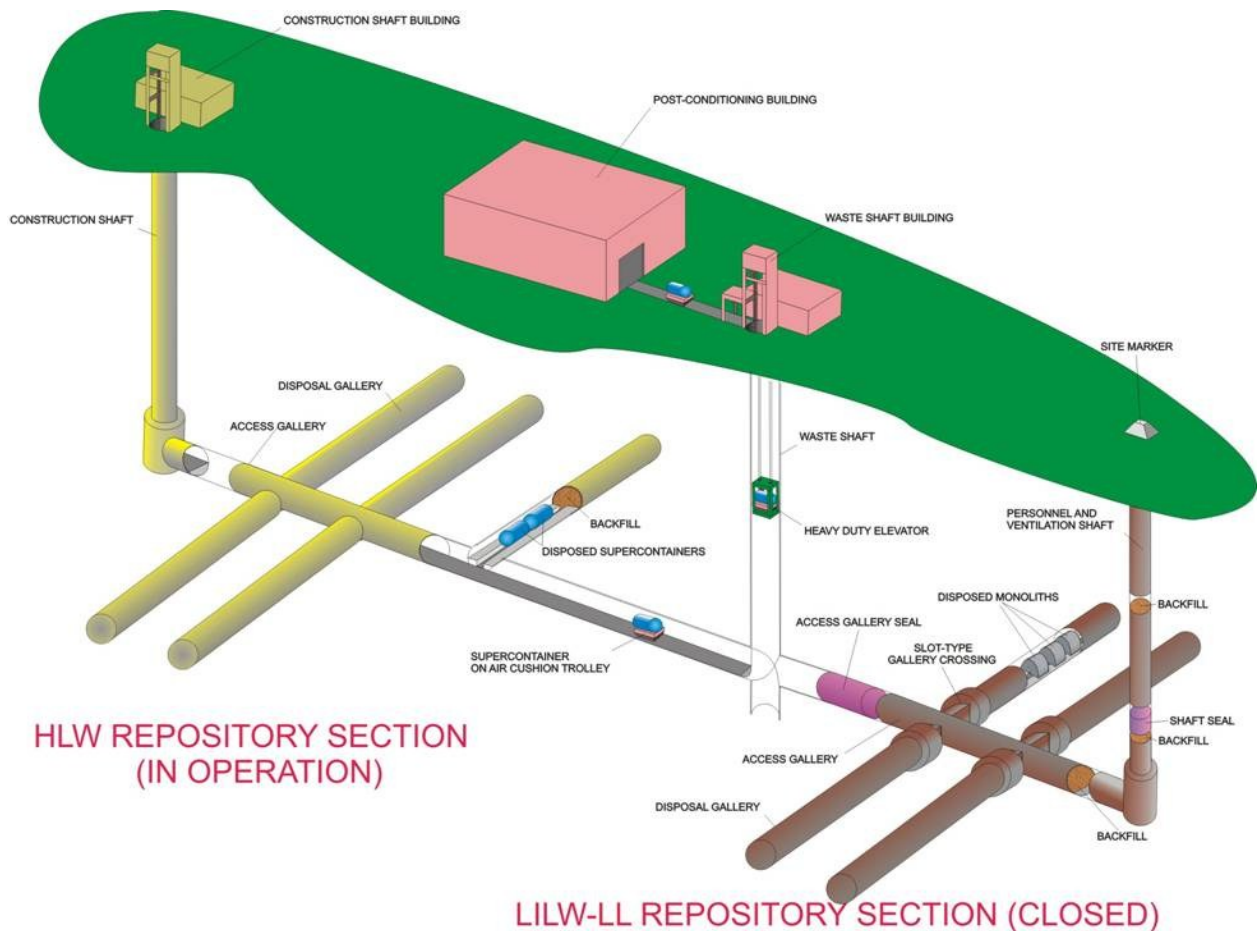


Figure 11: Lay-out of a geological disposal system for category B & C waste.

Separate sections are foreseen for disposal of category B and C waste. The waste packages (*i.e.* supercontainers or monoliths), will be emplaced horizontally one after the other (no distance in-between) in the centre of the disposal galleries. These galleries are drifts about 1 000 m long,

which are lined with concrete wedge blocks (gallery liners). Because the Boom Clay is a plastic clay, this concrete lining is required to limit convergence of the gallery walls. The considered backfill material, foreseen to fill the void space between waste packages and tunnel liners, is also based on cement. The thickness of the backfill will be between 40 to 50 cm for galleries filled with supercontainers, and only 10 cm for those filled with monoliths.

The distance between the axes of the disposal galleries will depend on the temperature limitations that are considered in the design study. Based on thermal calculations (Sillen and Marivoet, 2007), it is expected that a distance of about 120 m (spent fuel) and 50 m (vitrified-HLW) is sufficient to respect the maximum allowable temperature increase of the porewater.

In the case of UOX spent fuel, a total gallery length of about 14.2 km will be required for disposal of all the spent fuel containing supercontainers (see Table 11). When it is assumed that all spent fuel will be reprocessed, the total gallery length required for category C waste decreases to 6.5 km. Taking into account the compacted waste arising from reprocessing the spent fuel, the required gallery lengths become ~16 km (no further reprocessing) and ~8 km (full reprocessing).

Table 11: Required gallery length: comparison between the case of no further reprocessing (moratorium protraction) and the case of resumption of reprocessing activities.

	No further reprocessing gallery length (m)	Full reprocessing gallery length (m)
UOX spent fuel	14222.2	-
MOX spent fuel	792.0	-
V-HLW	792.7	6544.7
Total spent fuel + V-HLW	15806.9	6544.7
CSD-C waste	172.5	1387.5
Total	15979.4	7932.1

3.3 Geological host formation and surrounding geological layers

The Boom Clay in NE Belgium has been intensively studied since 1974 because of its favourable properties to host a geological repository for high- and intermediate-level radioactive waste. Boom Clay provides both a physical (limited water flow) and a chemical (retention) barrier for radionuclide transport. The very low hydraulic conductivity and the low natural hydraulic gradient over the formation make molecular diffusion the dominant solute transport process. A considerable fraction of the Boom Clay research has been founded on data obtained from the underground research facility HADES or its surroundings. Therefore, as a “working hypothesis”, the nuclear site of Mol-Dessel is currently considered by ONDRAF/NIRAS as the reference site for geological disposal.

The Boom Clay layer is a Tertiary formation belonging to the Rupel group, which has been sedimented during the Lower Oligocene, Rupelian Stage, between 28.4 and 33.9 million years ago. It consists of an alternation of silty clay and clayey silt, with a high content of pyrite and glauconite in the silty layers. The Boom Clay has a typical banded nature, with variations in silt

and clay content, carbonates (enriched in so-called septaria-bearing layers) and organic matter (Vandenberghe, 1978; Vandenberghe and Laga, 1986; Van Keer and De Craen, 2001).

The occurrence of the Boom Clay in Belgium is shown in Figure 12. The Boom Clay occurs in a rather continuous bed above an undulating east-west line running from the Scheldt estuary (Sint Niklaas region) to the Meuse (Eisden region) where it crops out. This outcrop zone is however interrupted in the region of Diest-Aarschot by an important (marine or fluvial) erosion channel formed during the Miocene by a strong coastparallel tidal flow (Wouters and Vandenberghe, 1994). The general dip of the Boom Clay is of the order of 1 to 2 % towards the north-east; its thickness increases in the same direction and reaches about 100 m in the northern Campine and beneath the reference site of Mol-Dessel. The geological structure at the Mol site is shown in Figure 13.

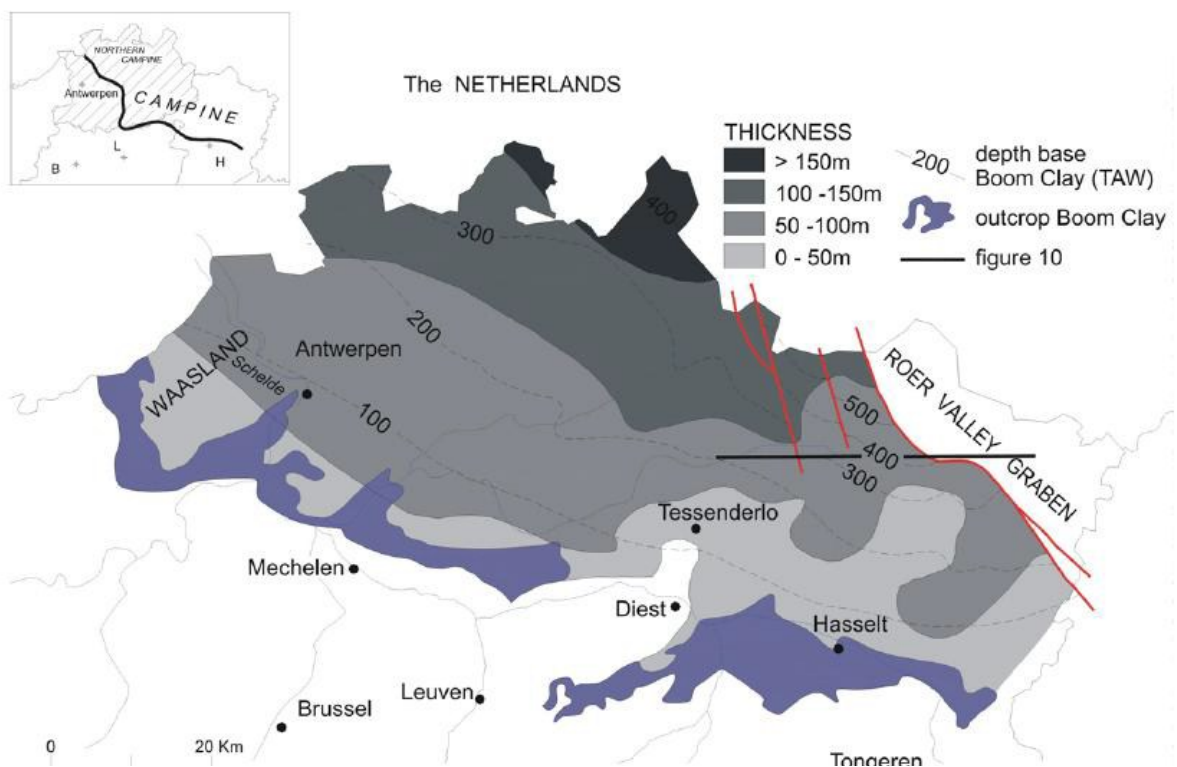


Figure 12: Occurrence of the Boom Clay in Belgium.

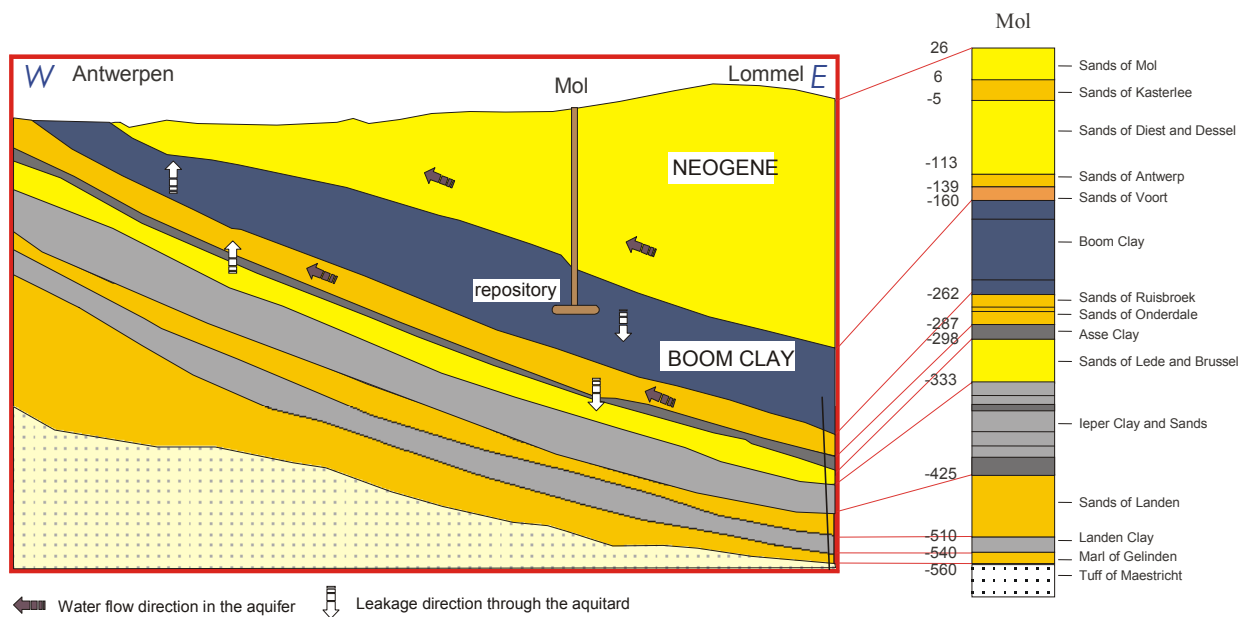


Figure 13: Geological cross-section at the Mol site.

Tertiary deposits form a regular sequence of alternating clay and sand layers where the Boom Clay is the uppermost main clay layer (see Figure 13). The main aquifer beneath the Boom Clay is composed by the formation of Lede and Brussel (sand and calcareous sandstone). This aquifer is overlain with the Maldegem Formation, containing the Asse Clay layer, which hydraulically separates the Lede-Brussel aquifer from the sands of Ruisbroek (Zelzate Formation) and Berg (Bilzen Formation). Together, they are often referred to as the Lower-Rupelian aquifer. This aquifer is not used as a water resource in the area considered for geological disposal, because it has a very limited pumping capacity.

The Boom Clay is overlain by the Oligocene sands of Eigenbilzen and Voort, belonging to the Upper Rupelian. Above the Oligocene, the Neogene aquifer starts which consists of the Berchem Formation (glauciferous fine sand, about 25 m thick) and Diestian Formation (about 100 m thick), containing the Diest sands (coarse sand) and Dessel sands (homogeneous fine sand), both glauconiferous. At present, the Neogene aquifer is intensively used as a regional water resource for drinking water production.

The Boom Clay is a detrital, fully marine deposit (Vandenberghe, 1978) and can be subdivided in four members (Belgian Subcommittee of Tertiary Stratigraphy, 2011):

- the Belsele Waas member represents the lower part of the Boom Clay, which is more silty and is characterised by two thick bands of silts and by the absence of organic matter horizons; the thickness is usually about 10 m;
- the Terhagen member represents the middle part of the Boom Clay which is the less silty part with two black bands rich in organic matter; the member thickness is about 20 m;
- the Putte member is the upper part of the Boom Clay, characterized by a systematic presence of black bands rich in organic matter and silty horizons; it has a maximum thickness of 40 m.

- the Boeretang member (formerly known as transition zone or 10WIG sequence). This member lies at the top of the formation, between 191 and 216 m BDT, and consists of alternating layers of silt and clay. Stratigraphically, it is related to the Putte member.

Regarding the migration of radionuclides, tests carried out on the Mol-1 cores for non- or slightly retarded species such as HTO (tritiated water), $^{131}\text{I}^-$ and HCO_3^- indicate that migration parameters vary little throughout the group that comprises the members of Boeretang, Putte and Terhagen and even the top few metres of the Belsele-Waas member as depicted in Figures 14 and 15. Meanwhile, these top few metres have been reclassified as belonging to the Terhagen member, so that the boundary between the two members is now a little deeper (Belgian Subcommittee of Tertiary Stratigraphy, 2011) The Boom Clay thickness considered in the safety assessment corresponds to the thickness over which the Boom Clay exhibits homogeneous radionuclide migration properties, *i.e.* 90 m, representing the Boom Clay zone between 191 m and 281 m BDT⁴, (Aertsens *et al.*, 2005). However, traditionally a safety margin is taken on the thickness so that the assumed Boom Clay thickness accounted for in the models of the reference case versions 1-3 is effectively only 80 m.

⁴ BDT: below drilling table

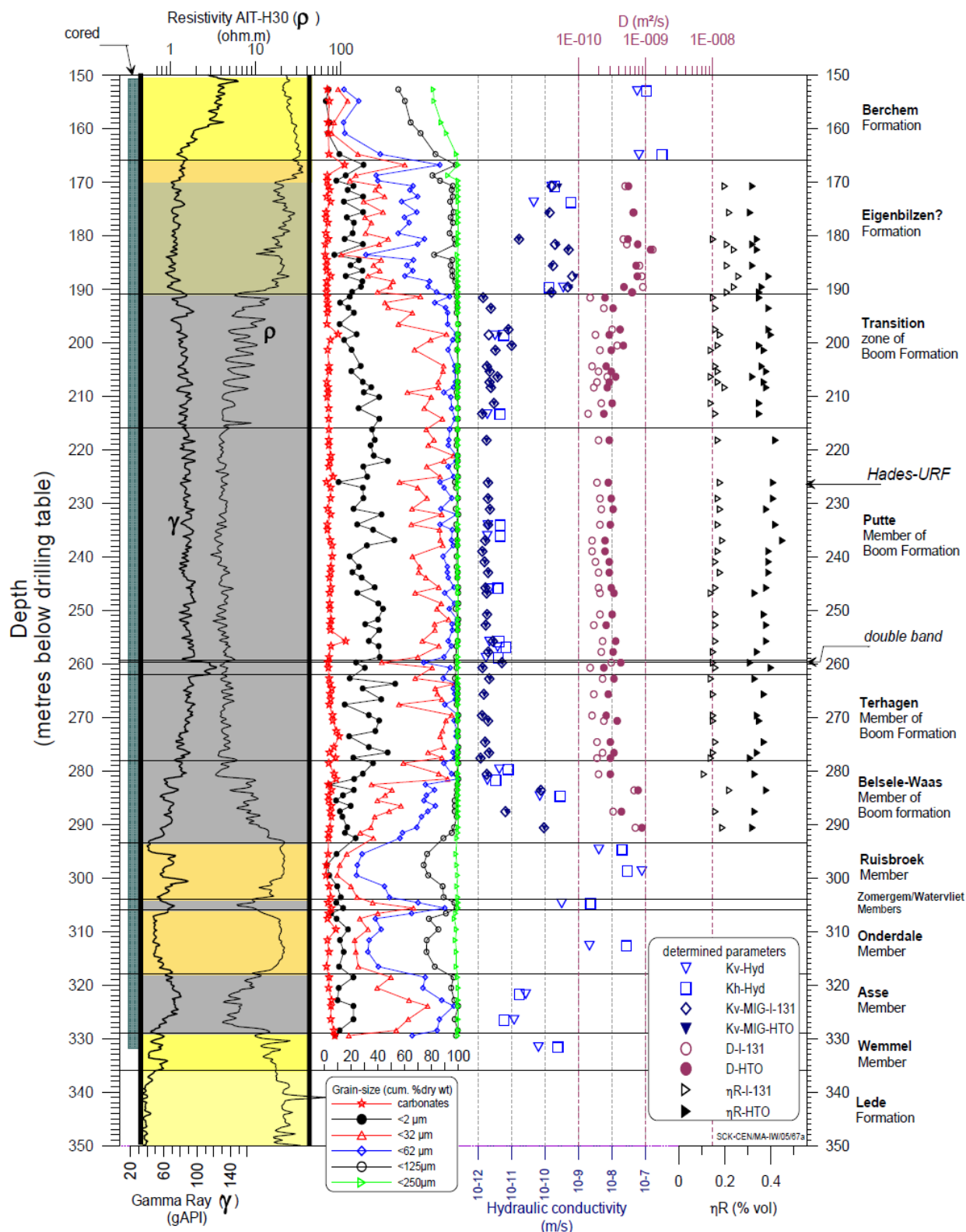


Figure 14: Vertical profile of hydraulic parameters in the Boom Clay and overlying/underlying layers for the Mol-1 drilling (May 1997): hydraulic conductivity, dispersion coefficient, ηR and water content W (source: Aertsens et al., 2005).

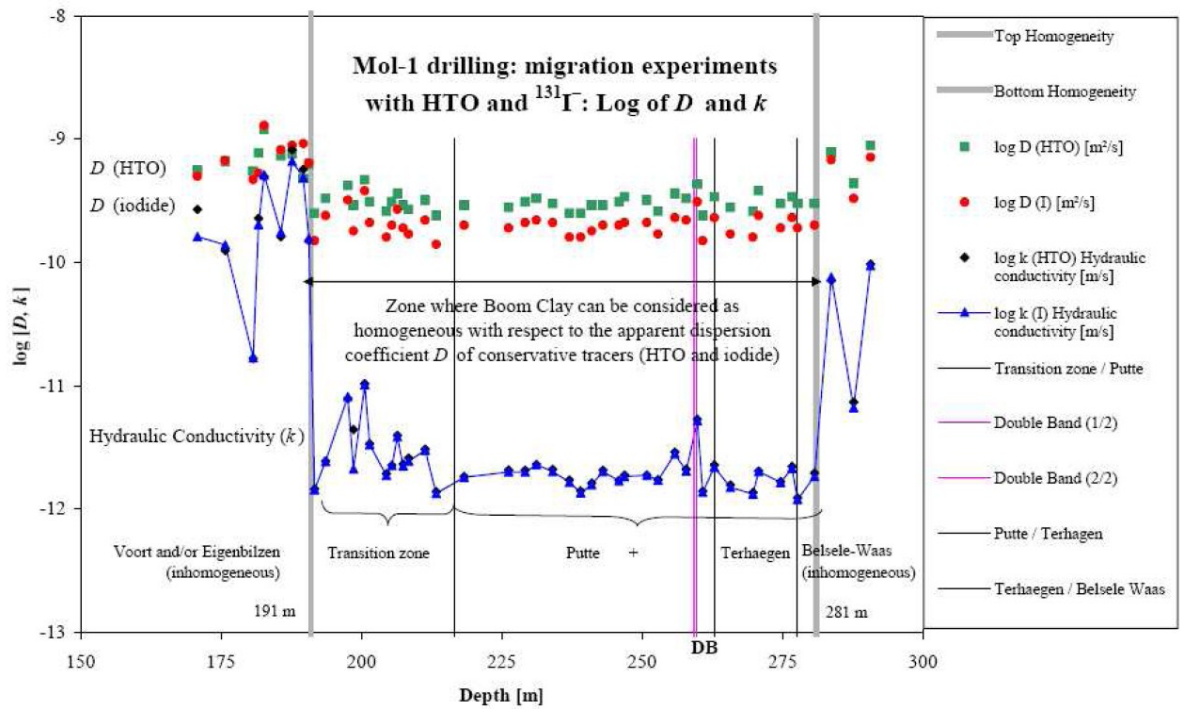


Figure 15: Vertical hydraulic conductivity and vertical apparent dispersion coefficient for HTO and I as a function of depth for the Boom Clay at the Mol site (MOL-1 borehole) (Aertsens et al., 2005).

4 The reference scenario

4.1 Definition of the reference scenario

The reference scenario is defined as the scenario corresponding to the safety concept (cf. section 1.2). It assumes that all safety functions are effective within the assigned time frames. This means that events and human actions having the potential to perturb the safety functions will not occur within the period covered by the assessment. Additionally, it is assumed that the disposal system and its components are built and installed according to design specifications, and that the components show no flaws.

The reference scenario is a broad description of the reference evolution of the disposal system. In the preparatory safety assessment phase, the effect of uncertainties is assessed by means of scoping calculations or sensitivity studies. In the formal safety assessment, if deemed necessary, uncertainties can lead to the creation of alternative cases under the reference scenario. Uncertainties undermining a safety function can lead to alternative scenarios (ONDRAF/NIRAS, 2009c).

4.2 Exposure pathways

The main safety indicator for a geological repository is the annual dose to a representative person⁵. Radionuclides released from the disposed waste can migrate by diffusion through the host formation and enter into the aquifer system where it is transported advectively. Contaminated groundwater can reach the biosphere via pumping wells or via drainage by the rivers or canals. In the biosphere, man can be exposed to radiation via ingestion, inhalation or external irradiation.

At present, the considerable recharge and the high hydraulic conductivity of its main sand layer (Diest Sands) makes the Neogene aquifer overlying the Boom Clay an important regional water resource for drinking water production, and agricultural and industrial applications. In the preparatory phase of the safety assessment, this aquifer is therefore considered the most important biosphere receptor, and the drilling of a wellbore the most critical exposure pathway. In the Mol area, the Neogene aquifer is drained by a dense network of rivers and canals. Two exposure pathways at the interface between aquifer and biosphere are considered in the preparatory safety assessments: (i) pumping of groundwater by a small self-sustaining community, and (ii) the natural discharge of groundwater into small local rivers. Water from the well and the river are assumed to be used as drinking water by man and cattle, and for irrigation. In a later phase of the safety assessments, a third exposure pathway, called the soil pathway, will also be evaluated. The soil exposure pathway assumes that contaminated groundwater reaches the soil zone in winter and that these wetlands are used for grazing cattle in summer.

The evolution of the aquifer and biosphere at the timescale relevant to geological disposal is highly uncertain. Therefore, these are treated in a stylised manner in ONDRAF/NIRAS safety

⁵ An individual receiving a dose that is representative of the more highly exposed individuals in the population (see Publication 101, ICRP 2006). This term is the equivalent of, and replaces, 'average member of the critical group' described in previous ICRP Recommendations.

assessment methodology (ONDRAF/NIRAS, 2009c). This approach is consistent with international approaches (NEA, 2004; NEA, 2012)

4.3 Safety and Performance Indicators

To assess the overall safety of a geological repository by means of simulations of the radionuclide release and transport, specific indicators are needed which are the outcome of model calculations and which can be compared with reference values. Such indicators are often called safety indicators. The most commonly used safety indicator is the effective dose rate. However, calculation of dose rates requires making assumptions on potential exposure pathways, including human habits and changes in the surface environment, for which the uncertainty substantially increases with time. Therefore, it is desirable to apply additional indicators, complementary to the dose rate, which are independent of the biosphere evolution. This approach allows to evaluate and confirm the long-term safety of the disposal system following the principle of multiple lines of reasoning (Marivoet *et al.*, 2010).

For the presentation of the results of the formal safety assessments of SFC1, the following set of complementary safety and performance indicators is proposed.

Safety Indicators (SI):

- Annual dose to a member of the potentially most exposed group. This is compared to the upper value of the dose constraint of 0.3 mSv/a as recommended by the ICRP (2000, 2011)
- Radiotoxicity concentration in aquifer water. A reference value of 20 $\mu\text{Sv}/\text{m}^3$ is assumed obtained from natural radiotoxicity concentrations in groundwaters from Finland, Switzerland and the Czech Republic (Becker *et al.*, 2003)
- Radiotoxicity flux out of the host formation. A reference value is assumed that was derived from data on the application of phosphate fertilisers in Flanders. (Marivoet *et al.*, 2010)

In the preparatory safety assessments, these indicators are tested, albeit not systematically in all calculation series. Various sensitivity studies on alternative models (processes) and on possible contributions of components are carried out for the development of the reference case. Therefore, the calculations are often limited to fluxes out of the host formation.

Performance Indicators (PI):

A performance indicator “provides measures of performance to support the development of system understanding and to assess the quality, reliability or effectiveness of a disposal system as a whole or of particular aspects or components of a disposal system” (IAEA, 2003). They aim at explaining the functioning of the repository system by quantifying the contribution of its main barriers (component-based PI) or safety functions (safety-function-based PI).

On the basis of the results obtained in the European projects SPIN (Becker *et al.*, 2003) and PAMINA (Becker *et al.*, 2009; Marivoet *et al.*, 2010), it is proposed to consider the following performance indicators:

- *Activity in compartments for a few key radionuclides, radiotoxicity in compartments for all fission and activation products, and radiotoxicity or number of moles in compartments for the 4 actinide chains.*
As it is expected that only a small fraction of the actinides will be released from the host clay formation up to 1 million years, it is important to clearly illustrate the evolution of the actinide inventory in the compartments of the disposal system during that period.
- *Integrated fluxes out of compartments: a few figures for key radionuclides and tables of the values after 1 million years for all relevant radionuclides.*
On the basis of the migration parameters considered in this study, small releases of actinides are expected before 1 million years. Therefore the calculations might be extended up to 10 million years for the reference case to better illustrate the behaviour of the actinides in the disposal system.
- *Performance indicators for safety functions, based on integrated fluxes.* These give in very compact way and in combination with the indicators activity/radiotoxicity/moles in compartments, an insight in the functioning of the disposal system.

When the preparatory safety assessments will be completed, the indicators will be reevaluated and, if considered necessary, the lists of indicators to be calculated in the formal assessments can be adapted.

The calculation procedure for these safety and performance indicators is detailed in 5.2.6.

4.4 Phenomenological evolution of the disposal system

A realistic analysis and the demonstration of an adequate level of understanding of the evolution of the disposal system are essential parts of the assessment basis of a nuclear waste disposal system. Indeed, the state of the disposal system at the time of radionuclide release represents the boundary conditions for the safety assessment calculations. Furthermore, it is important to demonstrate that near field processes as well as processes in the environment external to the disposal system (e.g. climate evolution, geological processes) do not significantly or irreversibly affect the favourable properties of the host formation as a barrier. In the case of Boom Clay, these favourable properties include a very low permeability, a small diffusion coefficient of dissolved solutes in the clay, a high retardation capacity, the absence of preferential migration pathways for solutes, as well as creep and swelling properties which result in a good self-sealing capacity.

The construction of the disposal infrastructure and operation of the repository, and the emplacement of heat-emitting radioactive waste, will inevitably induce thermal (T), hydraulic (H), mechanical (M) and chemical (C) disturbances of the Boom Clay. The repository system is also subject to radiological (R) and biological (B) processes. Among these processes, the thermal phase is considered the most severe disturbance that the repository system will undergo. To ensure that radionuclides are not released in a heated, and hence difficult to characterise repository system, IAEA recommends, and the ONDRAF/NIRAS' safety strategy requires that the overpack stays intact for at least the duration of the thermal phase (IAEA, 2006; ONDRAF/NIRAS, 2009a).

Although couplings between these THMC(B)(R) processes have been observed, they are discussed independently in the following sections. Potential interactions between the processes are indicated when considered important.

Apart from perturbations caused by “internal” processes, induced by the excavation of galleries and the introduction of foreign materials, the repository itself may be subject to “external” processes, due to other processes or events occurring mainly at the (sub)surface. The Boom Clay is very effective in buffering the repository from these (sub)surface events through the “isolation” safety function (I), but some processes could have a limited impact at repository depth. An example is the evolution of the climate in the long term (see discussion on thermal evolution in section 4.4.1). Apart from the climate evolution, it is not expected that radionuclide transport will be significantly influenced by these internal and external processes. As a summary, the main conclusions with respect to the reference evolution taken into account in the safety assessment are stated in paragraph 4.4.6. Remaining uncertainties that have the potential to impact the performance of the repository will be studied further and could be illustrated in alternative cases of the reference scenario or in altered evolution scenarios depending on the way they affect the safety functions of the disposal system. The proposed description of the reference case considers the current climate as a reference, but the impact of other climate states, which predominantly affect the aquifer and biosphere compartments of the safety assessment model, will be demonstrated in climate variants of the reference case.

4.4.1 *Thermal evolution*

Category C waste

Initially, the temperature at a certain depth is determined by the average surface temperature, the thermal properties of the stratigraphic layers and the geothermal flux. At the Boom Clay midplane at the reference site, the present temperature is about 16°C.

The principal heat source in the repository system is provided by decay of category C waste, but other sources including exothermic chemical reactions (short term) or drastic persisting temperature changes at the surface may also contribute to the heat budget. However, the heating effect of cement hydration reactions in the repository is expected to be minor because much of the concrete to be emplaced in the repository will have cured and cooled at the surface.

High-level radioactive waste generates considerable amounts of heat through radioactive decay. In the short-term, the radionuclide couples Sr-90/Y-90 and Cs-137/Ba-137m determine the heat production. After a few half-lives of Sr-90 and Cs-137 (both have a half-life of about 30 years), the heat production is determined by actinides (especially Pu-239, Pu-240 and Am-241). Since spent fuel contains the most actinides, the thermal phase⁶ is longer in the case of spent fuel disposal (Weetjens, 2010).

Waste loading and disposal density determine the required cooling time. After unloading from the reactor, spent fuel is allowed to cool down at the reactor site. Vitrified HLW will also need a cooling period. Currently, the cooling time considered for category C waste is 60 years after unloading from the reactor, irrespective of burn-up or glass fabrication time.

After the heat-emitting radioactive waste is emplaced and the repository is closed, the disposal system will undergo a severe transient period on a large spatial scale and in a relatively short period. Dissipation of the heat through the engineered barriers and Boom Clay is expected to occur mainly by conduction. The clay will conduct heat anisotropically with a thermal

⁶ For a definition of “thermal phase” in this context, see Sillen and Weetjens (2008).

conductivity of about 1.3 W/(m×K) in the vertical and 1.7 W/(m×K) in the horizontal direction (obtained from the ATLAS III *in situ* test, described in Yu *et al.*, 2011). As a result, the emitted heat from radioactive waste induces peak temperatures around 100°C in the buffer close to the overpack, and an extensive zone of elevated temperature in the clay with a peak of more than 70°C within 1-2 decades. This peak temperature depends on the properties of the waste, the design of the engineered barriers, and the spacing between the disposal galleries. The thermal disturbed zone will extend to the whole thickness of Boom Clay although the temperature change decreases rapidly with distance. The short term temperature evolution in the repository near field is shown in Figure 16. For spent fuel, a relatively "hot" spent fuel, with a burn-up of 55 GWd/tHM was selected to be conservative.

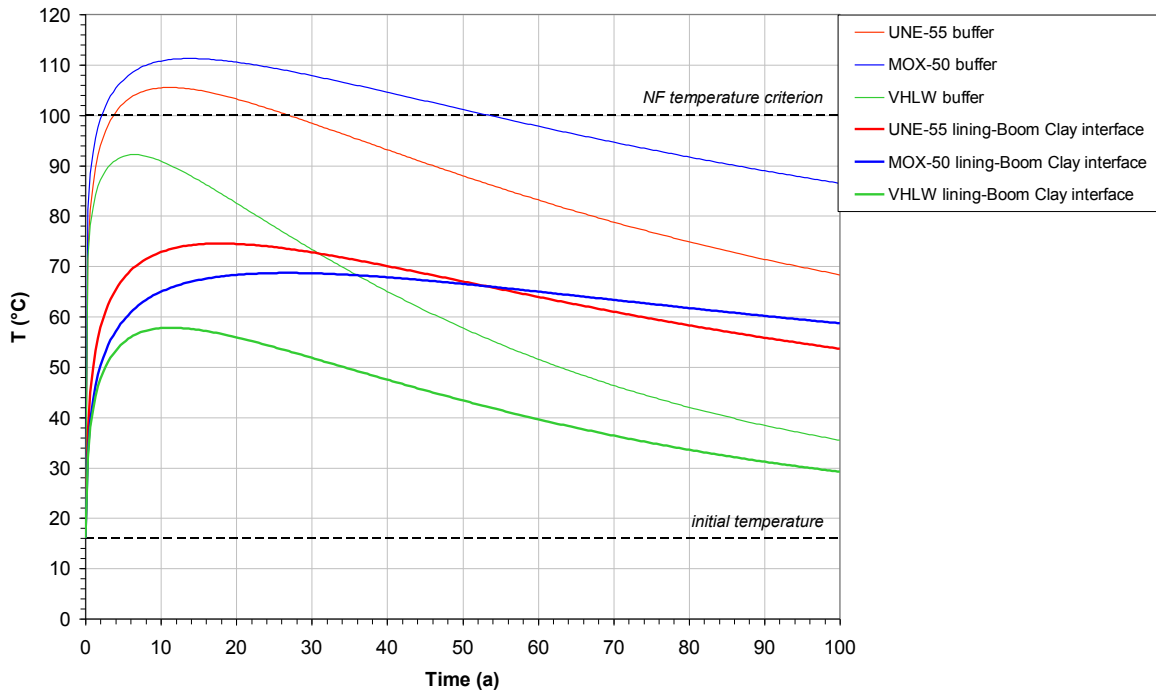


Figure 16: Temperature evolution in the Supercontainer buffer and at the interface between gallery lining and Boom Clay; disposal after a cooling period of 60 years. At the level of the overpack, a 3D anisotropic calculation with $\lambda_v=1.3$ W/(m×K) and $\lambda_h=1.7$ W/(m×K) is equivalent to a 2D axisymmetric calculation with $\lambda_{clay}=1.45$ W/(m×K).

ONDRAF/NIRAS is following an iterative approach in repository design which allows the disposal system to be designed in such a way that the thermal evolution is acceptable. At present, the maximum allowed temperature within the engineered barriers of a geological repository for heat emitting waste is set at 100°C. This limit was chosen from corrosion viewpoint. Sillen and Marivoet (2007) concluded that the temperature of the outer surface of the overpack would remain below 100°C only if the cooling period was 60 years or longer. However, detailed 2D axisymmetric calculations (Weetjens, 2010) show temperatures exceeding 100°C for spent fuel (Figure 16) and longer cooling times (or lower waste disposal densities, if possible) are suggested should the current near field temperature limit be maintained. Research is planned to study the effect of temperatures > 100°C on corrosion behaviour. At the interface between Boom Clay and the Neogene aquifer, the temperature increase will be maximum 10°C, occurring about 500 years after disposal (Sillen and Marivoet, 2007).

After the peak temperature has been reached, a slow recovery to the initial temperature follows. The expected evolution of the temperature increase (ΔT) at different distances above a disposal

gallery and below ground level is shown in Figure 17 for UOX spent fuel and in Figure 18 for VHLW.

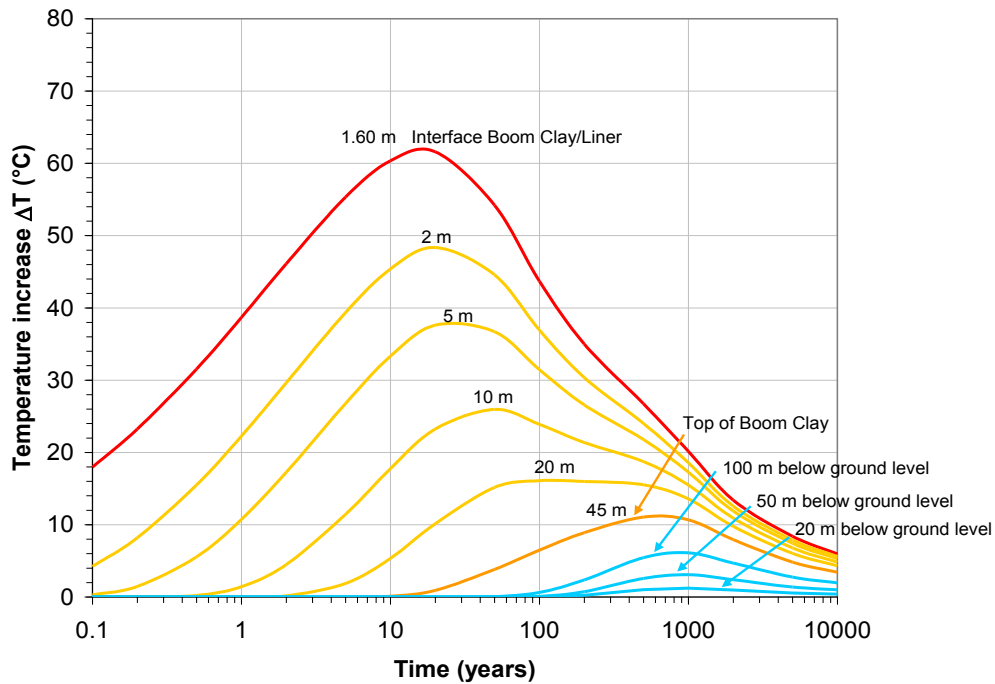


Figure 17: Time histories of temperature increase ΔT at various distances above a disposal gallery (orange) and below the ground level (blue), ENU55, disposal after a cooling period of 60 years, $\lambda_{\text{clay}}=1.35 \text{ W}/(\text{m}\cdot\text{K})$, $\lambda_{\text{aquifer}}=2.05 \text{ W}/(\text{m}\cdot\text{K})$; intensity of the source term spread over total supercontainer length.

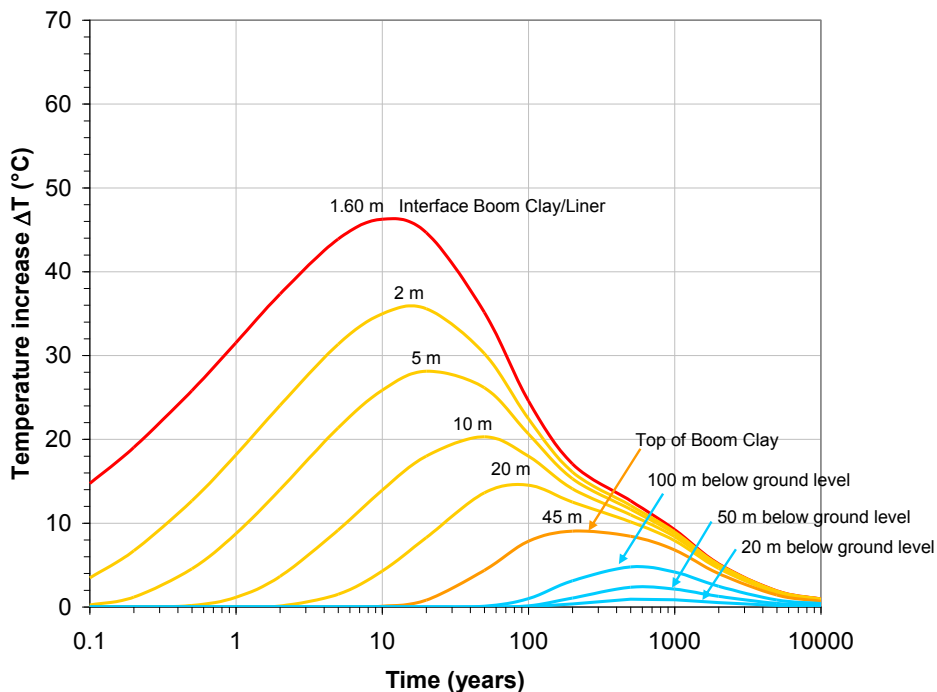


Figure 18: Time histories of temperature increase ΔT at various distances above a disposal gallery (orange) and below the ground level (blue), VHLW, disposal after a cooling period of 60 years, $\lambda_{\text{clay}}=1.35 \text{ W}/(\text{m}\cdot\text{K})$, $\lambda_{\text{aquifer}}=2.05 \text{ W}/(\text{m}\cdot\text{K})$; intensity of the source term spread over total supercontainer length.

The duration of the thermal phase can be derived from these figures. It is assumed that the values of migration parameters obtained from the laboratory are valid until 25°C, corresponding to an allowable temperature increase of 9°C. It is estimated that after 5000 years, the temperature of the host clay will have dropped below 25°C close to the engineered barrier system (EBS) in all cases. According to the ONDRAF/NIRAS strategic choices outlined in the safety strategy, it follows that, in the reference scenario, complete containment should be guaranteed by design for at least 5000 years. In the last decade, research on anaerobic corrosion of carbon steel in repository conditions has pointed out that uniform corrosion rates will be extremely small (<0.1 µm/year). In the hypothesis that uniform corrosion determines the containment time, this means that the overpack will remain watertight for a considerable longer time than is set out by the requirements.

The temperature at repository depth is assumed to be insensitive to changes in surface temperature. The expected increasing temperature in the short term (few hundreds/thousands years) is expected to have a limited impact on the behaviour of the disposal system, also considering that the overpack of the category C waste will be intact. On the long term, glaciations cannot be excluded (De Craen *et al.*, 2012). However, it is not expected that permafrost will reach the depth of the repository (Govaerts *et al.*, 2011). The possible impact of the permafrost climate state will be subject to further study to evaluate if this climate state has to be modelled in a specific calculation case.

The diffusion coefficient in the pore water is inversely proportional to the pore water viscosity and the latter decreases upon increasing temperature. Furthermore, an additional diffusive flux term may occur in response to a thermal gradient. This is known as the Soret effect. The direction of this mass flux, expressed by the Soret coefficient, depends on the relative directions of the temperature and concentration gradients.

However, an increase of diffusive fluxes due to temperature effects can be ruled out because radionuclides are still fully contained in the waste package during the thermal phase. A decrease of diffusive fluxes is possible in case of persisting permafrost conditions (the lowest calculated temperature at repository depth is 3°C; Govaerts *et al.*, 2011), but the nominal values of migration parameters obtained at 25°C in the laboratory can be conservatively applied in this case.

The heat flux from category C waste is not expected to cause effects on Boom Clay mineralogy. Smectite illitisation is known to be kinetically controlled by several physico-chemical parameters such as temperature and potassium-availability (Cuadros, 2006 and references therein). The temperature onset of smectite illitisation varies greatly in the literature from 70°C (Jennings and Thompson, 1986) to ~100°C (Inoue *et al.*, 1992) or more. The kinetics of the reaction is very slow at relatively low temperatures (a complete reaction would require several hundred Ma at a temperature of 80°C; Pytte and Reynolds, 1989). Moreover, the pore water chemistry in Boom Clay, being Na-dominated, is unfavourable for the advancement of the illitisation process (De Craen *et al.*, 2012). However, thermally induced CO₂ production from organic matter present in Boom Clay is possible. This effect is further discussed in §4.4.3.

For completeness, it can be mentioned that the waste heat production will promote microbial growth. However, to have microbial activity other conditions (notably availability of space and nutrients) need to be fulfilled. Research is ongoing to assess the effects of these processes.

Category B waste

For category B waste, which contains small amounts of Cs and Sr and much less actinides compared to category C waste, the design foresees no overpack; it is assumed that the waste disposal density is chosen such that the maximum allowable temperature change ($\Delta T=9^{\circ}\text{C}$) is not exceeded.

4.4.2 *Hydromechanical evolution*

During the excavation of the disposal gallery and shaft, a fracture zone is inevitably formed in the first meter of Boom Clay around the gallery as a result of the mechanical failure caused by stress redistribution. Beyond this fracture zone, an eye-shaped damaged zone with enhanced hydraulic conductivity due to effective stress variation is observed around the gallery into the Boom Clay up to 1.25-1.7 times the gallery diameter. The increase in hydraulic conductivity in the damaged zone is limited to one order of magnitude. No transmissive interconnected fracture network exists beyond a few centimetres into the Boom Clay. Furthermore, the fractures do not play an important role in the enhancement of the hydraulic conductivity in the damaged zone because self-sealing of the fractures occurs in a relatively short time. The permeability recovers close to the undisturbed value within a few years. In case of instant installation of the concrete lining, convergence can be limited to a few centimetres, thus further development of the fractures is effectively avoided. The consolidation under the hydraulic gradient towards the inner surface of the gallery and the confining pressure that develops upon fast installation of the liner, speed up the sealing process. The natural closing tendency of fissures and fractures is also related to the clay mineralogy. The use of a concrete lining and engineered barriers does not alter the sealing capacity of the Boom Clay. During the operational phase, ventilation of the repository induces limited desiccation in the clay formation close to the tunnel wall. However, the repository tunnels will be backfilled and closed soon after waste emplacement and the disposal galleries will become saturated with pore water fairly rapidly (within a few decades). Pressure equilibration of the repository's porous materials to *in situ* hydrostatic pressure proceeds more slowly, but equilibrium is assumed to be reached after a century (Weetjens *et al.*, 2006).

Category C waste

The hydromechanical behaviour of the disposal system is strongly coupled with temperature. For very low-permeable clay, the rate of temperature increase is generally more critical than the temperature itself to the potential thermal-induced mechanical effects on the clay surrounding disposal galleries. Due to thermal expansion of the porewater in the low-permeable host formation, increase of the porewater pressures is expected with an amplitude that depends on the interplay between the heat generation rate and the clay thermal and hydraulic diffusivities. The observed increase in hydraulic conductivity at elevated temperatures is entirely due to the decrease of the porewater viscosity, and hence is completely reversible. After the thermal transient period, the stress state and porewater pressure within the Boom Clay will recover slowly to their initial state. The heating-cooling cycle is expected not to alter the Boom Clay's pore structure. By the time of overpack breaching, the hydraulic conductivity is restored to its initial value and there is no hydraulic disturbed zone (Yu *et al.*, 2011).

Anaerobic corrosion of metallic EBS components will lead to the generation of hydrogen gas. Corrosion, although slow, will proceed for many hundreds of thousands of years. Depending on the amount of gas generated and the diffusion capacity of the clay, a free gas phase and associated gas pressure might build up in the repository. For category C waste, a free gas phase

may temporarily exist in the EBS and the saturation state at the time of radionuclide release remains somewhat elusive (Yu and Weetjens, 2011). However, it is not expected that the Boom Clay will desaturate or fracture due to gas generation. For the reference scenario, it is assumed that gas-driven radionuclide transport is negligible at all times, both in gas and liquid phase. Although subject to substantial uncertainty, most assessments to date indeed indicate that diffusive transport is expected to be sufficient to evacuate all generated hydrogen as dissolved gas (Weetjens and Sillen, 2006; Perko and Weetjens, 2011; Yu and Weetjens, 2011). The potential impacts of uncertainties related to gas generation and migration on the safety of the considered disposal system are still under investigation (*e.g.* in the EC project FORGE).

Category B waste

The gas generation rate in case of disposal of category B waste may be higher than for category C waste, since there is a relatively larger share in the amount of gas generation due to the waste itself, and due to the foreseen reinforcement bars in the monolith concrete. Exploratory calculations have shown that gas removal solely by diffusion would not be sufficient for the current disposal concept. Gas transport processes in low-permeability clay systems and EBS materials are currently being investigated in the FORGE project. At the national level, gas generation and migration for category B waste will be the topic of further RD&D. However there is confidence that design optimisation should be able to mitigate gas-related problems without affecting the system confinement properties. In the current reference scenario, it is assumed that the system has been iteratively designed such that the amount and rate of gas generated per metre gallery is acceptable and the potentially enhanced radionuclide transport through water expulsion from engineered materials (primarily the backfill) is negligible.

4.4.3 *Chemical evolution*

Prior to repository construction, the rocks and groundwaters at the repository location are assumed to be typical of the Boom Clay, a silty clay or argillaceous silt with pyrite and variable carbonate and organic matter contents. The more reactive mineralogical components of the Boom Clay are calcite, siderite and pyrite, which will control the concentrations of dissolved calcium and iron, and the redox potential of the pore water. The equilibrium pore water can be considered a dilute NaHCO₃ solution with relatively high concentration of organic matter, a *pH* of ~8.5 and a redox potential (*Eh*) of around -300 mV.

The excavation of the galleries and the introduction of cementitious materials introduce large chemical gradients in the repository near field. Furthermore, the equilibrium state of geochemical reactions varies with temperature, as do reaction rates. Elevated temperatures increase the solubility of most solids (with carbonates and sulphates as exception), decrease the solubility of most gases and increase reaction rates. Geochemical reactions such as mineral dissolution and precipitation could affect the chemistry of pore water and/or the stability of minerals in an irreversible way.

Oxidation

Oxidation effects are unavoidable during excavation and operation of the repository structures. Boom Clay is very sensitive to oxidation because of the presence of pyrite (FeS₂) and organic matter. Pyrite oxidation leads to release of H⁺, affecting the *pH* of the clay. Moreover, the production of sulphates and intermediate thiosulphates may be directly or indirectly detrimental to steel components. In the presence of sulphate reducing bacteria (SRB), these sulphates may be converted back to sulphides, which in turn could intensify corrosion of steel. It has been

demonstrated that oxidation of pyrite is a relatively fast reaction, but limited to the fracture surfaces in the EDZ (De Craen *et al.*, 2011). Ventilation of the galleries, and in-diffusion of dissolved oxygen, will not lead to additional pyrite oxidation, because the host formation is expected to remain water saturated with a significant hydraulic gradient inducing water flow towards the galleries. The oxidised zone of the Boom Clay is therefore limited to about 1 m around the galleries⁷

Oxidation also irreversibly affects the composition (hydrogen and oxygen index) of the organic matter in Boom Clay, in general leading to more oxygen-containing functionalised groups, shorter-chain aliphatic compounds and the release of small dissolved organic matter molecules (Blanchart, 2011). This increase in DOC was also observed in piezometer water samples in the HADES underground which were affected by oxydation (Van Geet, 2004; De Craen *et al.*, 2011).

As long as there are hydraulic gradients in the system, the corrosion-aggressive oxidation products will be transported by advection towards the gallery internals. After hydraulic equilibrium, they migrate by diffusion. By conservative numerical simulations (Govaerts and Weetjens, 2010; Wang, 2006) the bounding concentrations of various corrosion-aggressive species is calculated, but comparison with thresholds for localised corrosion is not straightforward. RD&D is performed to underbuild that realistic concentrations of aggressive species will not trigger localized corrosion phenomena. In the reference scenario, it is assumed that localised corrosion phenomena can be excluded and that corrosion occurs solely through passive dissolution.

pH evolution

The current repository design for category C waste consists of a supercontainer with a concrete buffer made of Ordinary Portland Cement (OPC). Freshly hydrated OPC contains highly alkaline materials such as portlandite, sodium/potassium hydroxides and calcium silicate hydrates (C-S-H). As a result, the equilibrium pore fluid of cement/concrete is highly alkaline (pH>12). The OPC concrete has been selected in combination with the carbon steel overpack, because its corrosion behaviour in the highly alkaline environment is well known. The external surface of the overpack will be fully passivated and localised corrosion phenomena are ruled out. As such, the geochemical conditions close to the overpack are conditioned and buffered by the massive amounts of cement, so that the engineered containment safety function can be guaranteed during the thermal phase and for a considerable period thereafter.

The use of large amounts of cement in the repository changes the geochemical conditions in the repository near field for more or less the entire assessment timeframe, so that Boom Clay equilibrium conditions are not expected in the vicinity of the waste. Boom Clay pore water will diffuse in and degrade the concrete phases only very slowly, and the following evolution is expected:

- Stage 1: a pH around 13.5, controlled by the dissolved alkalis (Na and K)
- Stage 2: characterised by a pH of 12.5, controlled by the solubility of portlandite (Ca(OH)₂)

⁷ Since the extent of the oxidised zone is correlated to the initial damaged zone, it is dependent on the excavated gallery diameter.

- Stage 3: a pH between 12.5 and 10.5, regulated by the equilibrium of C-S-H phases with the in-diffusion of Boom Clay pore water solutes
- Stage 4: the final stage is characterised by a pH lower than 10.5 but higher than 8.5, buffered by calcite ($CaCO_3$)

Geochemical model calculations showed that in case of the supercontainer concept, a pH of 12.5 (Stage 2) is predicted for a very long time at the overpack surface: it takes about 80 000 years before the pH starts to drop (see Figure 19; Wang, 2006). This calculation was very conservative since an infinite dilution boundary condition was directly applied at the concrete-clay interface, neglecting transport limitations in the Boom Clay.

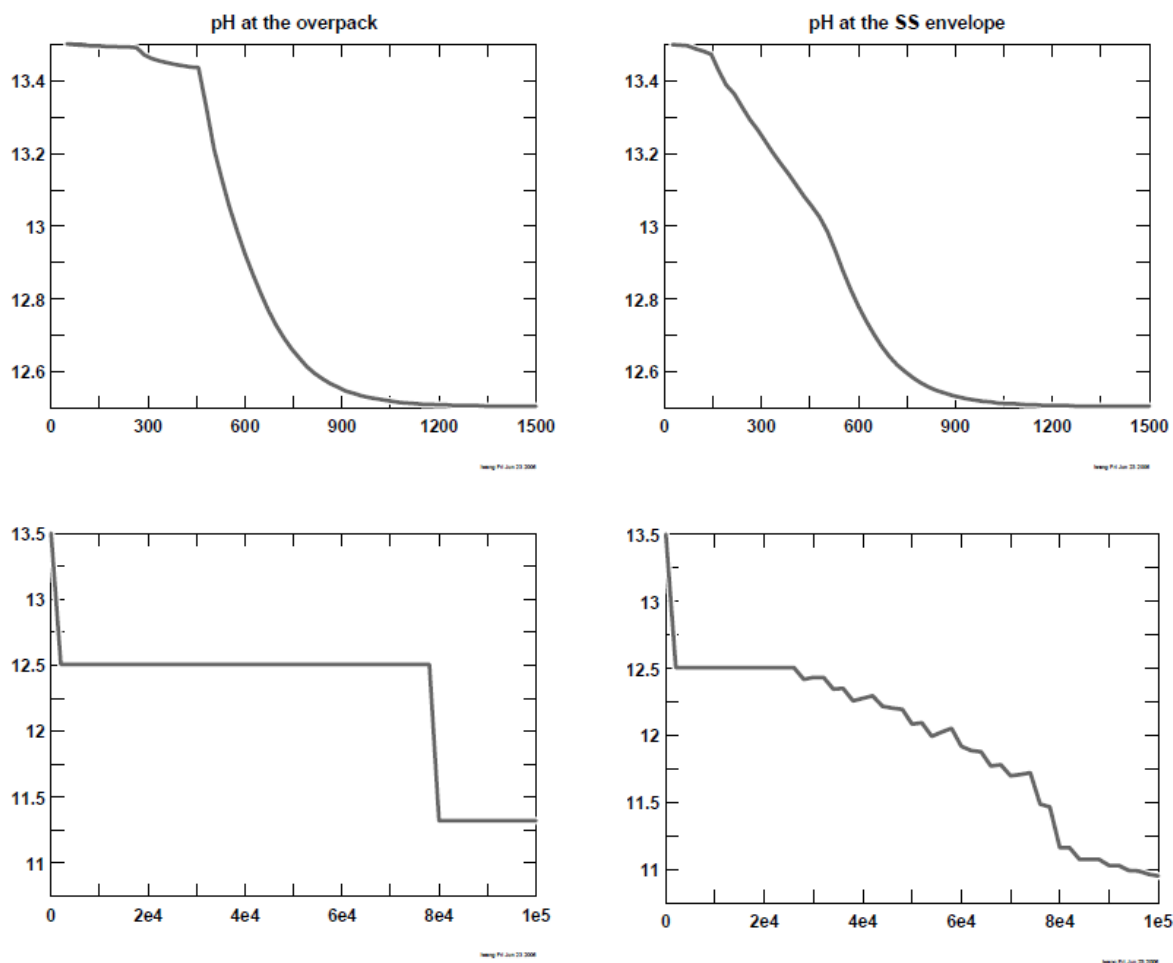


Figure 19: Evolution of pH at the overpack and the stainless steel (SS) envelope as a function of time (Wang, 2006).

A similar calculation including a certain volume of Boom Clay in the model led to an increase of Stage 2 duration to at least 100 000 years (see Figure 20; Wang *et al.*, 2009a).

In both calculations, an unrealistically low rate constant was applied to make calcite inert. In reality, calcite precipitation will occur as a result of calcium reacting with the in-diffusing dissolved CO_2 from the Boom Clay pore water. The thermal pulse through the clay even results in an increased dissolved CO_2 concentration in the vicinity of the repository due to release from organic matter (see further). Calcite precipitation could lead to pore clogging in the first centimetres of the buffer, so that the time needed for exhausting alkalis and portlandite would prolong substantially. As such, it is expected that in the reference scenario for category C waste,

the first two Stages will be dominant, although Stage 3 cannot be ruled out. The concrete buffer of the supercontainer is not expected to reach Stage 4 in the considered assessment timeframe of one million years. These geochemical models assumed a constant temperature of 25°C.

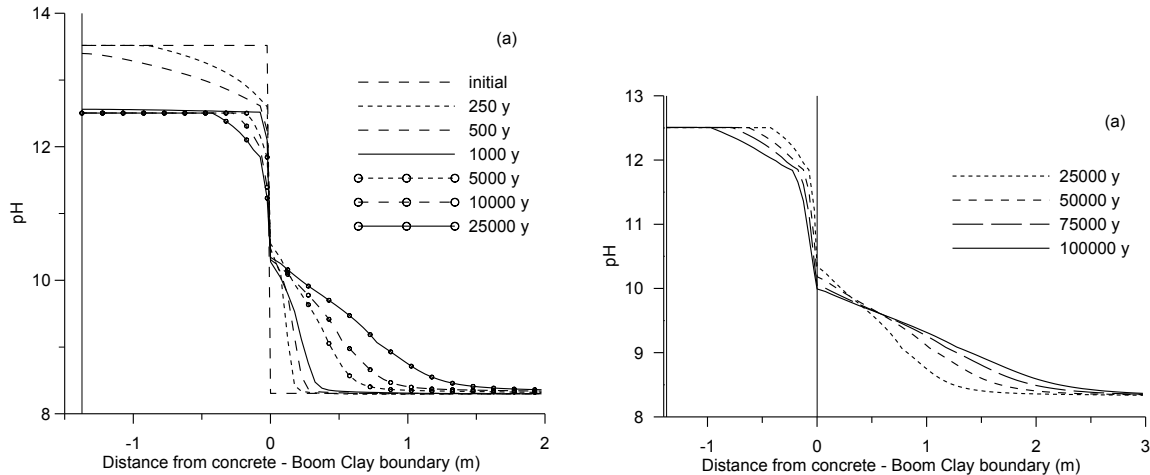


Figure 20: *pH evolution as function of the distance from the concrete – Boom Clay boundary in the short term (left) and long term (right).*

The *pH* evolution in the vicinity of the waste container (overpack) is a major pillar in the safety concept. The highly alkaline conditions will impose extremely slow uniform corrosion of the carbon steel overpack by passive dissolution. Furthermore, the evolution of the *pH* near the overpack also determines the geochemical conditions in which the waste matrices dissolve and (co)precipitation of radionuclide-bearing mineral phases will occur. In other words, the radionuclide release from the waste package depends largely on the expected *pH* evolution. In experimental programmes on waste dissolution, the presence of carbon steel and corrosion products is studied. The presence of hydrogen, produced by anaerobic corrosion of steel barriers is also taken into account in assessing spent fuel dissolution rates.

The integrated geochemical modelling of the concrete zone with the Boom Clay (Figure 20) also allows to assess the perturbation of the Boom Clay by the alkaline plume. A sensitivity analysis based on a supercontainer containing vitrified high-level waste shows that the spatial extent of the alkaline plume is limited to 2 – 2.5 m after 100 000 years. This is further supported by mass balance calculations. The combined effects of temperature and the alkaline perturbation on the THM behaviour during the thermal transient period is still somewhat uncertain, but it is not expected to significantly affect the clay's barrier properties. The extent of the damaged zone⁸ integrating all potential geophysical and geochemical perturbations of the host formation is estimated to be limited to 3 metres. In the safety assessment model, this uncertainty is conceptualised through definition of a damaged zone, in which there are no solubility limits and no sorption on Boom Clay minerals or organic matter.

⁸ Terminology corresponding to the definition by ONDRAF/NIRAS, in which the dZ is defined as “a zone of the host rock and its surrounding sediments where the values of any property are modified by the repository to such an extent that they have evolved beyond their nominal range” where “nominal range” is considered as a range of values representing state and properties of different components in undisturbed or initial conditions (ONDRAF/NIRAS, 2010)

It is assumed that the monolith concrete for category B waste is of similar composition as the supercontainer OPC-based buffer. The lower total mass of the concrete mineral phases per metre of gallery will lead to shorter durations of the subsequent degradation stages, and a smaller alkaline plume extent.

Organic matter and pCO₂ evolution

Compared to other argillaceous formations studied in the European context of geological disposal of radioactive waste, the Boom Clay contains substantial amounts of low-maturity organic matter (TOC content of 1 to 5%), distributed between the liquid and the solid phase. The organic matter found in Boom Clay is typical of its depositional environment during the Lower-Oligocene: clearly marine but with near-shore influences (Wouters and Vandenberghe, 1994).

A very small fraction (~0.05%) of the total organic matter content is in solution and is considered to be mobile. In a porous medium such as Boom Clay, the mobility of organic species in solution also depends on their molecular size, the largest molecules being immobilised in the pores by ultrafiltration. The cut-off equivalent to ultrafiltration is estimated to be 3×10^5 Da or about 20 nm. In the current phenomenological model it is assumed that all dissolved organic matter molecules smaller than this cut-off are potentially mobile and will not be filtered out by the Boom Clay. Furthermore, all mobile dissolved organic matter (DOM) is considered to show sufficiently similar characteristics and can thus be regarded as one homogeneous pool. DOM is considered in transport calculations as a colloidal phase, *i.e.* exhibiting a discrete charged surface that is able to interact with dissolved species/ions (Bruggeman and De Craen, 2012).

The insoluble kerogen fraction (~80% of TOC) is considered representative for the total organic matter pool in Boom Clay. Kerogen is a mixture of various nonpolymeric macromolecules, comprising both resistant biomacromolecules and recombined biodegradation products. Under the thermal stress that is expected for a repository containing high-level radioactive waste, kerogen is expected to release thermolabile components, which may change the chemical confining properties of the host formation. These thermolabile components are reactive oxygen-containing compounds of low molecular weight and will thus increase the mobile dissolved organic matter content.

Thermal cracking of the organic matter will also produce CO₂. Lorant *et al.* (2008) calculated a CO₂ production from 0.2 g/kg clay (at top of BC) to 0.6 g/kg clay (near the waste) based on a kinetic model⁹ and using the temperature data calculated in Sillen and Marivoet (2007). The released CO₂ might induce a chemical perturbation of Boom Clay pore water, resulting from a combination of three processes: (i) CO₂ production itself (acidification of pH), (ii) dissolution of carbonate minerals by H₂CO₃, and (iii) diffusion out of the heated zone of all species whose concentration is increased. For a given disposal configuration, the actual impact depends on the relative kinetics of these processes. In the near field, the CO₂-generating potential might become enhanced because of preliminary oxidation of natural organic matter due to gallery excavation.

Concerning the evolution of the *concentration* of dissolved organic matter (DOM), experts postulate that the following several processes may have an impact (Bruggeman and De Craen, 2012):

⁹ In this kinetic model, the bottom temperature or onset of the thermal cracking process is set to 20°C and the tests were performed on pure kerogen (Lorant *et al.*, 2008). The numbers mentioned are likely an underestimation since the presence of clay minerals and water may enhance the CO₂ production.

- Decrease of current *mobile* organic matter concentration in Boom Clay porewater due to diffusion to the aquifers
- Increase of the dissolved organic matter concentration in Boom Clay porewater due to alterations of the NOM pool subject to oxidation, heating and an alkaline plume. This replenishment of DOM from the solid phase will be primarily restricted to the near field.
- Increase of current mobile organic matter concentration in Boom Clay due to lixiviation of "anthropogenic" organic substances in disposal site (e.g., plasticisers in concrete, bituminised waste).

Concerning the *reactivity* of dissolved organic matter (DOM), experts postulate the following hypotheses based on experimental observations of similar behaviour for all humic/fulvic acids (Bruggeman and De Craen, 2012):

- All mobile organic matter generated/released under future evolution/perturbation conditions from the solid/immobile organic matter fraction will have the same general characteristics as the mobile organic matter in the porewater under the present conditions. This assumption is reasonable given that the source pool of organic matter for present-day and future dissolved organic matter is the same, and it is known from literature that humic acid/fulvic acid (HA/FA) pools in general have very similar characteristics.
- All anthropogenic organic matter also has the same general characteristics (complexing capacity towards radionuclides, transport as colloid, (limited) sorption/retardation, etc.) as the mobile organic matter in the porewater under present-day conditions. Therefore lixiviated anthropogenic organic matter is assumed to enlarge the pool of mobile dissolved organic matter with similar characteristics for radionuclide complexation.

The increase/decrease in mobile dissolved organic matter concentration that may be the result of future evolution/perturbation scenarios will be studied in the future, as well as the impact of the vertical variability of the organic matter. In the reference scenario however, constant organic matter concentrations and reactivity as present day are assumed for the whole assessment timeframe.

At the moment, porosity changes due to organic matter decomposition/structural changes are neglected.

4.4.4 *Biological evolution*

The construction of the repository can change the environmental conditions in the vicinity of the galleries which may induce bacterial activity:

- A temporary porosity increase of the disturbed zone and small residual voids in the EBS may provide space for bacteria to grow
- Introduction of oxygen changes chemical balances and various contaminations (from waste itself or stray materials from engineering operations) in and around galleries may provide additional nutrients
- Bacteria may be introduced by cross-contamination and manned operations

In the longer term, it is expected that environmental conditions are harsh for bacterial growth. After backfilling and repository closure, oxygen will be depleted fairly quickly and conditions become reducing. The use of small-porosity engineered barriers and the fast convergence and

self-sealing of the Boom Clay will make space limited. In addition, the near field will become very alkaline due to the use of OPC-based concrete in supercontainer or monolith, backfill and gallery lining, and for high-level waste the near field will make a temperature excursion well beyond 70°C. Nevertheless, the scientific community is convinced that some bacteria are able to survive in these extreme conditions, although it is unknown if they are active. However, it is expected that bacterial activity would be very low: nutrients and metabolites will have to be transported respectively to and from the bacteria by diffusion. This puts an effective limit to their activity and growth.

In view of long term safety, sulphate reducing bacteria (SRB) may play an important role. Sulphates, produced by oxidation of pyrite during the operational phase, may be reduced back to sulphides by SRB, and these may in-diffuse into the supercontainer buffer where they may induce localised corrosion phenomena on the carbon steel overpack, thereby undermining one of the principal hypotheses of the safety concept. Currently an RD&D programme is investigating whether sulphide thresholds (in combination with other aggressive species or not) for localized corrosion are higher than what can realistically be expected from SRB activity. Other bacteria, such as methanogenic bacteria, may play a positive role. Some methanogens, called hydrogenotrophic methanogens, use carbon dioxide (CO₂) as a source of carbon, and hydrogen as a reducing agent. The volume of gas produced by anaerobic corrosion of steel barriers or auxiliary components may then be reduced by a factor of 4, which reduces significantly the risk of overpressurisation or gas-driven radionuclide transport.

In the reference scenario, localised corrosion phenomena are assumed to be excluded and potential positive effects of microbial activity are not taken into account in view of robustness of the assessments.

4.4.5 Radiological evolution

Radioactive decay will produce helium gas (alpha decay) and radon gas (mainly owing to decay of ²²⁶Ra, itself a daughter product of the ²³⁸U decay chain). In the short term, these gases are produced inside the overpack where they accumulate with other fission gases. From a hydromechanical point of view, they are not considered significant compared to the hydrogen generation due to corrosion.

The radioactive waste will create a radiation field in and around the repository, whose intensity will decrease over time. The gamma radiation field from the waste can alter the geochemistry and to a lesser extent the mineralogy of the near field (Noynaert, 2000; Noynaert *et al.*, 1998) and might also generate gas due to radiolysis of pore water (Bouniol, 2005). The generation of various oxidizing species may significantly increase the redox potential close to the overpack and this effect may last for about 300 years (Bouniol, 2007). The impact of radiolysis on anaerobic corrosion of carbon steel in alkaline media was investigated in an experimental programme. For radiation levels below 25 Gy×hr⁻¹, the long-term anaerobic uniform corrosion rate of carbon steel seems to be independent of the radiation dose rate (Kursten, 2012).

4.4.6 Summary: reference evolution in performance assessment

The description of the phenomenological evolution provides boundary conditions and support for ensuring that the safety functions are effective. Concerning the reference evolution considered in

the (preliminary) safety assessment, the key conclusions for the post-containment period can be summarized as follows:

- There are no lasting effects expected of THM-related perturbations on the Boom Clay matrix structure. At the expected time of overpack failure, the porosity, density, permeability and pore diffusion coefficients are assumed to have recovered to their initial, undisturbed values.
- The direct (*e.g.* alkaline plume and pCO₂ evolution) and indirect (*e.g.* irreversible thermal effects on Boom Clay organic matter reactivity with respect to radionuclide complexation: changes in concentration, size distribution and functional groups) chemical perturbations of the clay are somewhat uncertain. These perturbations will affect the sorption characteristics, organic matter interactions and solubility in the near-field, but are not expected to significantly change the far-field geochemistry. In the safety assessment model, this uncertainty is conceptualised through definition of a disturbed zone, limited to a few metres, in which there are no solubility limits and no sorption on Boom Clay minerals or organic matter.
- The *pH* evolution of the concrete barriers will affect the release from the waste form (R1 safety function) in two ways: it will determine the waste dissolution rates and the near field solubility. *pH* evolution is described by four successive Stages (from *pH* = 13.5 to *pH*<10.5).
- In the reference scenario, gas-driven radionuclide transport is assumed to be negligible at all times in both the gas and liquid phases. For high-level waste, the risk of gas problems is limited, although (partial) desaturation of the EBS cannot be excluded. For category B waste, gas generation rates are likely to be higher, resulting in a higher risk for pressure build-up and structural failure of barriers and/or Boom Clay. As a premise, it is assumed that design measures are taken to avoid this situation or that, in any case, it would not lead to enhanced radionuclide transport.

4.5 Evolution of the environment of the disposal system

The two components of the environment of the disposal system, *i.e.* the aquifer system and the biosphere, are expected to change considerably with time. At short time scales (decades), human habits and food production techniques can already strongly influence the biosphere. At longer time scales (centuries) the aquifer system and the biosphere will be affected by climate changes. In accordance with most European safety assessment methodologies (NEA, 2004; NEA, 2012), an approach based on stylised biospheres and aquifer systems will be used (ONDRAF/NIRAS, 2009c).

The environment of the disposal system will be influenced by climate change. The following approach has been adopted for SFC1 (De Craen *et al.*, 2012, and references therein) in which five main time frames are distinguished:

- The period 0-10 ka:
 - Overall, this period is characterised by a climate similar to or moderately warmer than at present and with a similar degree of water availability through the year, though with drier summers.

- If global warming is not limited, flooding of the Mol-Dessel area by the sea cannot be excluded. This could have a moderate impact on the disposal system but a drastic effect on the environment. Salt water could intrude into the aquifers surrounding the host formation and this could affect the transport properties of the clay and the overpack lifetime. Coastal and marine erosion processes would flatten out the existing topography.
- The period 10-50 ka:
 - Relatively warm conditions are expected to continue since most climate models predict the presence of a long interglacial ahead.
 - One model (BIOCLIM A3) predicts a slow and gradual transition to a glacial maximum shortly after 50 ka AP. This, together with the fact that long interglacials are not very common during the Quaternary period, justifies that a cold climate without permafrost should also be considered during this period.
- The period 50-170 ka:
 - Interglacial conditions are expected to continue, but cold intervals are possible
 - Ice cap development is not expected in northern Belgium in this time frame.
- The period 170-400 ka:
 - All BIOCLIM models predict glacial maxima in this timeframe, hence cold climate conditions are expected, including permafrost development during strong glacial maxima.
 - Ice cap development is not expected in northern Belgium in this time frame.
- The period 400 ka-1 Ma:
 - All BIOCLIM models predict glacial maxima of high intensity (with permafrost) alternated with relatively warm interglacial periods
 - Ice cap development is not expected in northern Belgium in this time frame.

It is not realistic to forecast the evolution of the climate over the next 1 Ma. Therefore, in the reference scenario and for the time frames defined above, stylised hydrogeologies and biospheres corresponding to the following climate types will be considered:

- current climate (all timeframes)
- global warming without marine transgression (all timeframes)
- global warming with marine transgression (all timeframes)
- cold climate without permafrost (boreal) >10ka
- cold climate with permafrost >50ka

The possible impact of these 5 climate states on the safety of the disposal system and its environment will be studied in the framework of uncertainty evaluations due to evolving conditions and may give rise to alternative cases of the reference scenarios or altered evolution scenarios.

5 The reference case

The reference case is a realisation of the reference scenario with a specific conceptual model and parameter dataset based on the state-of-the-art knowledge. It can be considered a simple, robust and defensible conceptual representation of the reference evolution that still upholds the safety concept. It is iteratively developed and tested using limiting values of the expert range. In this report, the description of the reference case is limited to the conceptual model description of the corresponding performance assessment model. Although some parameter data are mentioned in the document to scope the discussion, they are not thoroughly discussed since the process for data selection and the data themselves are still being iteratively refined in the current stage of preparatory safety assessment.

The present version of the reference case specifically considers the reference site of Mol. It is assumed that the disposal system and its environment evolve as described in Chapter 4. Section 5.1 and 5.2 outlines the conceptual and the mathematical model respectively.

5.1 Conceptual model

The reference model considers radioactive decay during the whole assessment period, all-at-once overpack failure after the containment phase, radionuclide release from the waste forms, radionuclide migration through the near field (engineered part of the disposal system and the disturbed zone of the host formation) and far field (undisturbed host formation). Radionuclides may undergo precipitation/dissolution reactions in the near field and/or far field. Some radionuclides may react with dissolved organic matter present in the (undisturbed) Boom Clay depending on their affinity to form complexes with organic matter. A small fraction of the radionuclides may eventually reach the surrounding aquifer layers, where they may become accessible to the biosphere. How these processes are conceptualised in the reference model is discussed below, structured according to the safety functions. The mathematical model is described in section 5.2

5.1.1 *Isolation (I)*

In the reference scenario, it is assumed that no events (including human intrusion) will have the potential to damage or bypass a safety function. In the reference case, we postulate that the climate and geology will be the same as today's conditions. In other words, no external events (erosion, sea water intrusion) will occur that might affect the barrier thickness, the depth or the properties of the host rock assuring the confinement. These effects will be investigated in the next step, where uncertainties due to evolving conditions will be evaluated.

5.1.2 *Engineered containment (C)*

Category C waste types

The Supercontainer design was developed based on the Contained Environment Concept, the aim of which is to establish and preserve a favourable chemical environment in the immediate

vicinity of the metallic overpack, so that it will be exposed to essentially unchanged, benign conditions for a long time, at least for the duration of the thermal phase. The backbone of the corrosion RD&D strategy, which aims to provide confidence that the overpack will remain intact for the required timeframe, is based on demonstrating that (i) corrosion will occur uniformly by passive dissolution, and (ii) no localised corrosion mechanism (*e.g.* pitting corrosion, crevice corrosion, stress corrosion cracking) can occur under the high *pH* conditions prevailing within the supercontainer (“exclusion principle”). The methodology followed consists of three phases (Kursten, 2012):

- Phase 1: Development of the Corrosion Evolutionary Path (CEP), taking into account the changing conditions (temperature, degree of saturation, Eh/*pH*) inside the supercontainer buffer.
- Phase 2: Determination of scientifically well-founded estimates of corrosion rates, based on both literature data and a corrosion experimental programme specifically dedicated to supercontainer conditions. Under these conditions, the carbon steel overpack is expected to undergo uniform corrosion through the mechanism of passive dissolution.
- Phase 3: Demonstrating the validity of the “exclusion principle”. Depassivation is possible due to *e.g.* ingress of aggressive species, which may result in localised corrosion attack such as *e.g.* pitting corrosion, crevice corrosion or stress corrosion cracking. Conservative supporting calculations (Govaerts and Weetjens, 2010; Wang, 2006) show that the maximum concentration of chlorine is still far below the potential threshold for localized corrosion in anaerobic conditions. The calculated thiosulfate (direct impact on corrosion) and sulphate (indirect impact if reduced to sulfides) concentrations are not expected to pose a threat for inducing localised corrosion.

In the reference case, it is assumed that localised corrosion phenomena will not take place, although the assessment basis for the “exclusion principle” is not (yet) well developed. This hypothesis, together with the deterministic nature of passive corrosion makes it rather straightforward to predict the overpack lifetime¹⁰, based on knowledge of the corrosion rate and the thickness necessary to withstand the *in situ* stress. This “mechanical” thickness is estimated at 15-20 mm, leaving at least 10 mm of the overpack thickness to resist corrosion, the so-called corrosion allowance layer. Weldings are assumed to be of good quality, with no enhanced susceptibility for localised corrosion.

The *pH* evolution is one of the dominant environmental parameters in the corrosion evolutionary path. During the first stage, the *pH* will be about 13.4, controlled by the dissolution of alkalis. In view of the requirement on overpack lifetime determined by the thermal phase, these conditions are indeed the most relevant, especially close to the overpack. Therefore, the corrosion experimental programme focuses on corrosion rates determined in presence of young concrete water (YCW). The experimentally determined corrosion rates in these conditions are very low, implicating that the containment phase could extend well beyond the thermal phase. By that time however, the *pH* in the vicinity of the overpack may have gradually evolved towards Stage 2 (*pH*=12.5), which is predicted to last more than 80 000 years. This will not influence the validity

¹⁰ The most recent assessments indicate an overpack lifetime of at least 100 000 years, *i.e.* much longer than the safety requirement that the overpack should remain intact during the thermal phase (in the order of 5000 years maximum). However, since the containment time depends on the corrosion rate and mechanical thickness (both the result of a data selection procedure), its value may be further iterated during the preliminary safety assessment phase. Discussions on the selected parameter values are out of the scope of the present report.

of the corrosion rate values, since the chemical conditions are still situated in the passive corrosion domain.

During the containment phase, the radionuclides in the waste will decay. After perforation of the overpack, the waste will come into contact with porewater and slowly begins to dissolve. It is assumed in the reference case that all overpacks breach at the same moment (no spreading in time of radionuclide release). Furthermore, overpack breaching is assumed to be complete, *i.e.* the breached overpacks provide no physical barrier to water ingress or diffusion of radionuclides. In reality, even in a degraded state the overpack still provides some barrier to release of radionuclides. No delay is considered in the start of spent fuel (SF)/high level waste (HLW) canister corrosion, due to the potential occurrence of a gas phase in the near field. Similarly, spent fuel cladding (e.g. Zircaloy-4 cladding 550-800 μm thick; Boulanger, 2011b) and vitrified HLW canisters (5 mm thick stainless steel) are not considered to provide an additional period of complete containment following overpack breaching.

The same overpack lifetime is assumed for all supercontainer variants (UOX SF, MOX SF and vitrified HLW), although the minimal mechanical thickness depends on the overpack diameter. Accordingly, the corrosion allowance layer will vary per waste type. Furthermore, the overpack internal elements (e.g. full cast iron insert keeping the assemblies in place) are not assumed to provide mechanical support to the overpack.

Category B waste types

According to the safety concept for category B waste (see Figure 2), no engineered containment phase is foreseen for these waste types.

5.1.3 Limitation of radionuclide releases (R1)

The radionuclide source term is given by the radionuclide release model, which determines how fast radionuclides will dissolve from the solid phase to the liquid phase and, hence, will become available for diffusive transport. Two processes contribute to this safety function:

- a) The slow dissolution of the waste form provides a general resistance to radionuclide release
- b) In addition, the release of some radionuclides is limited by their solubility

When the overpack loses its containment function, pore water can come into contact with the waste. Stainless steel canisters, assembly boxes and other internals are assumed not to form a barrier to water ingress, and the waste starts to dissolve.

In general, it is assumed in the assessment calculations that radionuclides released from the waste forms enter “reservoirs” of water within the SF and HLW canisters, and within the pore space of the emplacement tunnels, where they are uniformly mixed (imposed by the use of a very high diffusion coefficient). Chemical equilibrium is assumed to exist within the reservoirs.

Immobilisation by co-precipitation with secondary minerals derived from SF, glass and canister corrosion is conservatively neglected, as is sorption on the corrosion products of the canisters

and waste forms. The transport resistance provided by internal spaces (fractures) within the waste forms, by the breached SF/HLW canisters and by corrosion products is neglected¹¹.

a) **Waste form dissolution**

Waste dissolution processes in a repository environment are very complex and extensive research programmes are dedicated to this field of research. Although most trends and influencing factors are known, modelling these processes is not straightforward. Therefore, fairly simple waste dissolution models are used in the safety calculations. These are described below.

UOX Spent fuel (based on Lemmens, 2011a)

The radionuclide source term originating from spent fuel dissolution consists of three parts:

- (i) A slow release of radionuclides embedded in the fuel matrix. These are assumed to be released congruently and at a constant rate (constant matrix release model).
- (ii) The release of radionuclides from the cladding and structural materials. These are assumed to be released congruently and at a constant rate following cladding corrosion.
- (iii) A fast release of radionuclides, which are not embedded in matrix or structure, called the Instant Release Fraction (IRF).

(i) Matrix release

A constant matrix release model can be expressed as fractional release rate (y^{-1}) of which the inverse gives the duration of matrix dissolution. The fractional release rate can be directly measured (for a realistic geometry/surface area) or is obtained by combining a surface-normalised release rate with the surface area for dissolution. Both factors are assumed to be constant in the model.

The fuel matrix release consists of a sum of oxidative dissolution and non-oxidative dissolution terms. Oxidative dissolution occurs in oxic conditions, but can be triggered even in anoxic deep groundwaters by oxidative radiolytical molecules. The radiation dose level that determines the transition between oxidative and non-oxidative dissolution is referred to as the α -threshold. This threshold is reached sooner in reducing conditions, and therefore depends on the hydrogen concentration, which can reach significant levels due to anaerobic corrosion of steel barriers.

In the reference case, it is assumed that only non-oxidative dissolution occurs, based on two rationales¹²:

1. The radiation dose for UOX spent fuel decreases in time until the α -threshold is reached. The overpack lifetime is very likely to exceed that time.
2. Scoping calculations indicate that the dissolved hydrogen concentration in proximity of the spent fuel is sufficient to suppress oxidative dissolution. These H_2 levels are attained relatively soon after waste disposal and will persist for several hundreds of thousands of years.

¹¹ The use of “effective surface area” however does include assumptions on the transport resistance of internal fractures

¹² In experimental set-ups dedicated to measurements of non-oxidative dissolution, it seems that oxygen cannot be totally removed. Therefore the resulting values for the dissolution rates are slightly (but conservatively) biased.

The matrix release mechanisms in highly alkaline conditions are the same as in neutral conditions and the fractional release rates do not seem very *pH* dependent.

The specific surface area is assumed to be constant, although a slight decrease in time is expected. The influence of fuel burn-up seems to be small. The effect of external and internal stress development, which could cause breaching and increases the fuel surface area, is considered to be negligible. The external stress load is a result from lithostatic stress, thermal expansion/contraction phenomena, volume changes with respect to corrosion products and other mineralogical transformations. Internal stresses could result from He pressure, and volume changes due to secondary phase formation. However, the latter is more pertinent to the mechanism of oxidative dissolution.

The presence of fillings in contact with spent fuel has not been taken into account while assessing fuel dissolution rates. Various alternatives, mainly Ca-based minerals, are still under investigation. Sand is avoided as filling material because it creates uncertainties with regards to the possible formation of coffinite (uranium (IV)-silicate), which might increase the oxidative dissolution rate of the spent fuel.

(ii) Cladding and structure release

The radionuclide (activation products) release from cladding and structural materials starts at the time of overpack failure. The release is assumed to occur congruently with cladding/structure corrosion. The corrosion rate is assumed to be constant and is based on zircaloy corrosion in conditions as close as possible to the repository. With a given cladding thickness (550 μm), corrosion lifetime can be estimated, typically in the order of tens of thousands of years. The structural parts are assigned the same corrosion lifetime, although the thickness may differ.

Experts identify also a sudden release term originating from the oxidised part of the cladding corresponding to 20% of the cladding inventory. This is not included in the SA calculations of version 3 of the reference case.

(iii) Instant Release Fraction

The radionuclide fraction, located in fuel microstructures for which no confinement properties are anticipated or can be demonstrated at the time of containment loss, is assumed to dissolve instantaneously, and is called Instant Release Fraction (IRF). This fraction is radionuclide-specific, and is assumed to dissolve instantaneously. These radionuclides are mainly present in the gap between fuel and cladding and in the readily accessible grain boundaries. The radionuclides in the rim pores and grains, and in the metallic inclusions in the fuel matrix are considered as a potential IRF, but these compartments are expected to be less accessible. The radionuclides in the oxidized zone of the cladding are also considered as IRF, although in reality, they may be released slowly.

The IRF depends not only on the distribution of the radionuclides within the spent fuel after discharge from the reactor (IRF at $t=0$), but also on the intrinsic evolution of the spent fuel before overpack failure. However, there is reasonable evidence that this extra term to account for diffusion of radionuclides to the grain boundaries during the containment period is negligible. In other words, the IRF considered corresponds to the initial IRF.

The IRF increases with burn-up. In order to assess its impact, two reference burn-ups are considered for SFC1: 50 and 60 GWd/tHM. The safety calculations considered in the current reporting period (*i.e.* version 1-3) are limited to the 50GWd/tHM reference fuel assembly. In a

next step, the impact of higher burn-ups on the IRF, as well as the additional IRF fraction from the oxidised part of the cladding will be studied.

MOX spent fuel

MOX fuels have been studied much less intensively than UOX fuels. The mechanisms and models of fuel dissolution are assumed to be the same. The only clear difference pertains to the IRF.

The structure of MOX is different from UOX. The rim zone is not restructured to the same extent for MOX as for UOX, but MOX contains Pu-rich agglomerates with a high local burn-up and porosity. The most important compartments that contribute to the IRF are the gap, open grain boundaries and the Pu-rich agglomerates. The (radionuclide-specific) IRF values selected for the safety assessments of SFC1 can be considered initial values representative for MOX fuel with a burn-up of 50 GWd/tHM (Cachoir and Mennecart, 2011).

Vitrified HLW (based on Lemmens, 2011b)

Glass dissolution is assumed to start immediately after overpack failure. Radionuclides embedded in a vitrified waste matrix are assumed to leach congruently with glass dissolution. Selective leaching is not expected to be an important process, since it may only become rate-determining at $\text{pH} < 11.7$ (at room temperature).

A process-level model for glass alteration in repository conditions exists, with the most important processes being the following:

- Selective release of soluble glass components
- Hydrolysis of the glass matrix
- Gel formation and evolution
- Silica saturation of the solution
- Precipitation of secondary phases
- Radionuclide retention in gel and secondary phases
- Removal of Si from the solution by advection, diffusion or sorption

Although this process-level glass dissolution model and the experimental data on relevant timescale suggest a decrease of dissolution rate with time, the model proposed for the safety assessment calculations is constant. Similar to spent fuel dissolution, the waste dissolution time is determined by two factors, both considered constants: the glass alteration rate (in this case SON68 borosilicate glass) and the cracking factor, used to calculate the effective surface area.

A high pH environment tends to decrease the gel density and its protective properties. Hence, the glass alteration rate increases with pH . The values selected for the reference case correspond to glass dissolution in Young Cement Water ($\text{pH}=13.5$). Irradiation does not seem to be a key factor affecting glass dissolution and it is therefore not taken into account in the reference case.

The net evolution of the effective surface area is difficult to predict. Cracks may close due to precipitation of secondary phases, and the surface area will also decrease as the glass dissolves. On the other hand, reopening of cracks or even formation of new cracks cannot be excluded, e.g.

by internal/external stress development but these are believed to be limited. In the reference case, the surface area is assumed to be constant.

Category B waste (CSD-C)

Fission products and actinides are expected to be on the surface of the cladding and therefore they are assumed to be released immediately. On the other hand, the activation products are generated in the cladding material and they are assumed to be released congruently with the cladding corrosion. A possible additional instant release originating from the oxidised zone of the cladding is not considered in the current reference case version.

b) Near field solubility limits

Solubility limits may contribute to the R1 safety function by limiting the dissolved concentration of the concerned radioelement. For most radionuclides, the solubility in a high-*pH* near field condition (imposed by the large amounts of cement) is similar or even lower than in the geochemical conditions imposed by the Boom Clay. A few may show higher solubilities in the high-*pH* near field. However, near the waste the radionuclide concentration will be the highest, depending mainly on the inventory, the release rate from the waste and the diffusion rate into the host clay. Hence, the contribution of solubility limitations to the confinement of radionuclides is the most effective in the vicinity of the waste form.

The solubility limits near the waste are strongly determined by the prevailing geochemical conditions (Eh and *pH*). The *pH* around the waste will undergo several stages as explained in section 4.4.3. As the overpack lifetime is expected to be considerably longer (10–100 ka) than the design requirement (5 ka), determination of the near field geochemistry at the time of waste dissolution is not straightforward. Furthermore, there is little experimental basis for determining the concentration limit in the considered conditions. The parameter selection for radionuclide solubility therefore relies mainly on thermodynamic calculations. Much effort has been spent on the quality of the thermodynamic database and selection of the most probable mineral phases. Seetharam *et al.*, (2011) made a review of the radionuclide solubilities for the cementitious near field of the planned surface disposal facility for category A waste in Dessel (Province of Antwerp, Belgium). For the selection of the solubility values, the *pH* state of the cement based material (see above), as well as the concentrations of the main cations in a particular cement state, were taken into account. Selected solubilities were either taken from reliable experimental data or from thermodynamic modelling, by assuming equilibrium of a solubility controlling phase with the simulated cement pore water. It should be noted that the solubilities for the surface waste disposal facility are often values for oxidising conditions. For the redox-sensitive radionuclides, these values are usually higher than for the reducing conditions that are expected in a geological repository.

In the preliminary safety assessment, scoping calculations have been performed taking the effect of near field solubility into account (notably in reference case version 3, see section 6.3). The following assumptions were made:

- Amorphous phases are also considered and even preferred to crystalline phases in the data selection process although the latter are thermodynamically more stable on the long-term. Solid solution and co-precipitation processes are not considered.

- Due to substantial uncertainty on near-field conditions, the highest solubility value of concrete degradation Stages 1-3 is conservatively applied (incl. 95% confidence interval).
- An exception was made for U, for which the solubility limit was restricted to Stages 1-2 in view of consistency with the chosen non-oxidative release model.
- The precipitation/dissolution of radionuclide bearing minerals is assumed to be an instantaneous process. Any impact due to precipitation/dissolution processes on the porous nature of the domain is not considered.
- The selected solubility data are implemented as a fixed value (no time evolution) and are assumed to remain valid over the whole assessment timeframe.
- The concentrations of the most important stable isotopes in the waste (Se and Pd) are taken into account.
- The solubility limits of the different isotopes (e.g. uranium) is obtained from the product of the isotope fraction in the waste and the solubility limit of the element. The influence of the temporal evolution will be evaluated in the future.
- The near field solubility limit is applied at the waste/concrete interface.

5.1.4 Limitation of water flow (R2)

Radionuclide transport through the near field and the Boom Clay layer is essentially due to molecular diffusion. This is supported by the low hydraulic conductivity and the fine, homogeneous pore structure of Boom Clay, the low hydraulic gradient over the host formation (0.02 to 0.04 m/m at the reference site), as well as the backfilling and sealing of the access tunnels and shafts. In the reference case, the sealed access tunnels and shafts are assumed to provide no preferential transport pathways at any time as defined by the reference scenario (no safety function bypass).

The Péclet number illustrates why convective and dispersive transport can be neglected in the Boom Clay:

$$Pe = \frac{u_{Darcy} \cdot x}{D_{eff}}$$

with $D_{eff} = \eta D_p$

where Pe (-) is the Péclet number, u_{Darcy} (m/s) is the Darcy water flux, x (m) is the distance, D_{eff} (m²/s) is the effective diffusion coefficient, η (-) is the porosity and D_p (m²/s) is the pore diffusion coefficient. For $Pe \ll 1$, diffusion dominates strongly over advection at the distance x from the source. Given that Boom Clay beneath the Mol-Dessel nuclear zone is characterised by a very low vertical hydraulic conductivity ($K_{vert} = 2.1 \times 10^{-12}$ m/s) and natural hydraulic gradient (3 m head of water over 100 m thickness of clay), radionuclide migration is essentially controlled by diffusion, with advection playing a limited role, since Pe is less than 1 in all cases¹³. Therefore, the reference case does not take advective transport of radionuclides and other contaminants into account. Scoping calculations showed that in the current hydrogeological situation advection causes a small increase (about 5%) of the radionuclide fluxes to the lower (Under-Rupelian) aquifer and a small decrease to the upper (Neogene) aquifer (Liu *et al.*, to be published). Omitting the advection term in the reference case is thus conservative.

¹³ For example, iodine is characterised by a D_{eff} in Boom Clay of the order of 2.3×10^{-11} m²/s. Then, Pe is equal to 0.13 at the Boom Clay formation boundary ($x = 50$ m, $K_{vert} = 2.1 \times 10^{-12}$ m/s, hydraulic gradient = 0.03, $u_{darcy} = 6.3 \times 10^{-14}$ m/s).

Excavation, construction and operation of a repository will cause physical and chemical perturbations to the surrounding host rock and create a “disturbed zone” (dZ) or even damaged zone (DZ). In the reference case, by the time of overpack breaching, the hydraulic conductivity is expected to be restored to its initial value and there is no hydraulic disturbed zone. Potential hydromechanical effects due to gas generation are not considered in the reference scenario (see reference evolution in chapter 4). Therefore, the DZ considered in the safety assessment calculations represents chemical perturbations rather than hydraulic perturbations.

5.1.5 Retardation and spreading in time of radionuclide migration (R3)

Radionuclides dissolved from the waste form or near field precipitate will diffuse through the engineered barriers, towards the Boom Clay, where they may interact with minerals and organic matter. The near field is assumed to be fully water saturated at that time. Migration through the saturated porous media concrete and clay is assumed to be well represented by the well-known advection-dispersion-reaction (ADR) equation (see paragraph 5.2.2), where the advection term is negligible as guaranteed by safety function R2 in the reference scenario. In this conceptual model, particularly adequate for diluted systems, sorption is assumed to be linear and reversible (so-called K_d approach). All transport paths from the repository through the host rock are assumed to be identical in their transport-relevant properties, *i.e.* the porous media are assumed to be homogenous and isotropic. A distinction is made between radionuclide migration through the near field (engineered barriers and disturbed zone of Boom Clay) and radionuclide migration through the far field (the undisturbed Boom Clay).

Radionuclide migration through engineered barriers and disturbed zone

The radionuclides that enter the liquid phase become available for diffusive transport. Some radionuclides sorb on the cementitious barrier and auxiliary materials present in the near field. This may even be the case for some radionuclides that are not retarded in Boom Clay (Govaerts *et al.*, 2012e). Wang *et al.* (2009b) made a review of the R_d values¹⁴ of radionuclides for the cementitious near field of a surface radioactive waste disposal facility in Dessel. For the selection of the sorption values, the *pH* state of the cement based material, as well as the main solid phases (still) present at that state, were taken into account: state I ((Na,K)OH): $13.5 > pH > 12.5$; state II (Ca(OH)₂): $pH \sim 12.5$; state III (CSH): $12.5 > pH > 10$; state IV (calcite): $pH < 10$. The mentioned R_d values in Wang *et al.* (2009b) were determined for cement paste. Transferability of these data to concrete barriers in geological disposal conditions is not yet investigated, and especially potential concrete mineralogy transformations due to the thermal evolution composes a source of uncertainty. Hence, although radionuclide sorption on cementitious components may account for a safety reserve, notably for category B waste, it is conservatively neglected in the reference case for all considered wastes. Indeed, the evolution of concrete degradation in geological disposal conditions is still poorly characterised, especially when subject to a severe thermal transient.

The same applies for the disturbed zone of Boom Clay, which is the zone of Boom Clay that suffered from excavation damage and geochemical perturbations affecting radionuclide transport. The observed fast self-sealing capacity of the Boom Clay prevents lasting alterations of the clay structure (Bernier and Davies, 2005; Bernier *et al.*, 2007; Yu *et al.*, 2011). However,

¹⁴ R_d (ℓ/kg) is a general term for distribution ratio suggesting that equilibrium may not be achieved, and that the linearity and reversibility of the sorption process are not yet demonstrated. In this report, the term K_d (ℓ/kg) is rather used to denote the distribution ratio, *i.e.* the ratio between adsorbed concentration C_s (kg/kg dry solid) and the liquid phase concentration C_l (kg/ℓ)

the geochemical perturbation caused by the alkaline plume (and by other near field effects, e.g. oxidation, pCO₂ increase due to thermal decomposition of kerogen) may be considerable. The extent of this perturbation is assumed to be smaller than 3 metres in the reference case (see also paragraph 4.4.3). In this zone (damaged zone according to the O/N definition), radionuclide reactions or interactions such as (co)precipitation, complexation with natural organic matter and sorption processes cannot be reliably accounted for.

Hence, in the reference case it is assumed that radionuclides and contaminants migrate through the engineered barriers and disturbed zone as conservative tracers. Radionuclides are not solubility limited in the DZ.

Radionuclide migration through Boom Clay

Radionuclide retention and transport in Boom Clay has been intensively studied for more than 25 years. Based on these results and on chemical analogy considerations, groups of radionuclides have been outlined that show similar geochemical behaviour under far-field disposal conditions. Parameter value ranges are proposed that are consistent with phenomenological models that have been drafted for each group. These phenomenological models combine all available knowledge from thermodynamic sources, experimental batch data and (different types of) migration experiments. The proposed value ranges are valid only for Boom Clay in the reference site Mol-Dessel (current geochemical conditions) and take into account the vertical variability throughout the formation.

Based on state-of-the-art knowledge, the following conceptual model for radionuclide migration in Boom Clay is proposed in the framework of SFC1.

The Boom Clay is considered homogeneous in its transport behaviour, and contains no discontinuities that are relevant to radionuclide transport and retention. Anisotropy of diffusion is not taken into account in the reference case because its impact on the total flux released into the aquifers is negligible. The influence of horizontal features (e.g. septaria layers) and the Boom Clay's anisotropy on radionuclide transport is verified by supporting calculations (Liu *et al.*, to be published).

The safety-relevant radionuclides are grouped according to their similarities in chemical behaviour (speciation, sorption, transport) under Boom Clay reference conditions. These similarities and differences allow delineating groups of elements for which the behaviour is sufficiently similar to use the same phenomenological model: (i) neutral and anionic radionuclide species; (ii) cationic radionuclides; and (iii) radionuclides that can form complexes with natural organic matter. The migration parameters provided by the experts for these groups are listed in Table 12 (Bruggeman *et al.*, Integration report draft version, 2011).

Table 12: Migration parameters required for the conceptual model that is proposed for the considered radionuclide group, with η [-] diffusion accessible porosity, D_{app} (m²/s), D_p (m²/s), R (-) retardation factor defined as $R=1+(\rho_b \times K_d)/\eta$, k_{decomp} the decomplexation rate, K_{comp} the thermodynamic complexation constant, c_{OM} the concentration of dissolved organic matter, and η_{OM} and $D_{app,OM}$ the diffusion accessible porosity and apparent diffusion coefficient for dissolved organic matter respectively.

	η	D_{app}	D_p	R	k_{decomp}	K_{comp}	c_{OM}	η_{OM}	$D_{app,OM}$
Neutral (HTO)	×		×	×					
Anions	×		×	×					
Cations	×	×		×					
NOM linked RN	×		×	×	×	×	×	×	×

The groups (and respective phenomenological models) that are considered as well as the assignment of the radionuclides to the different groups are outlined hereafter:

1. The first group comprises only the reference conservative tracer HTO, and is not further discussed for the purpose of this report.
2. A second group is made up by the anions, containing mostly non-metal elements from groups IVa to VIIa in Mendeleev's table. The reference element for this group is iodine (as iodide, I⁻). Se is also considered part of this group, both as the oxyanion selenate (SeO₄²⁻) and as the biselenide anion (HSe⁻). Indeed, selenate is considered to be metastable in the Boom Clay redox conditions, *i.e.* if Se leaves the near-field environment in this form, it is considered to be stable despite the redox disequilibrium with the reducing BC. Other elements belonging to this group are carbon (C, as bicarbonate, HCO₃⁻), chlorine (as chloride, Cl⁻) and Nb as Nb(OH)₆⁻. The anion group is characterised by limited or no sorption/retardation and due to the anion-exclusion phenomenon, the diffusion accessible porosity is reduced compared to HTO.
3. The third group consists of alkali and alkaline earth metals that are not hydrolysed under Boom Clay conditions. These metals are predominantly adsorbed through ion exchange and their transport is influenced by surface diffusion processes. Two subgroups are distinguished. The first subgroup with the monovalent metals Cs and Rb have a small hydrolysed radius and are preferably bound to so-called frayed edge sites (FES) in micaceous clay minerals such as illite. These cations also do not have a solubility limit. The second subgroup contains divalent cations that may form aqueous complexes with CO₃²⁻ and that are solubility-limited by the formation of carbonate phases. They preferably bind to the interlayer ion exchange sites of smectite minerals.

The use of (expert or source) ranges for the values of the retardation factor and D_p will result in an accumulation of conservatism and thus overestimation of the uncertainty on the migration behaviour. To avoid this problem, the value for D_p is calculated using the retardation factor and D_{app} . The obtained parameter combination is then always consistent with the given uncertainty range of D_{app} , which is considered the most robust and trustworthy parameter for describing the migration of cationic species in Boom Clay. The uncertainty on the migration of cationic species is thus completely determined by the range of the D_{app} values.

4. The fourth and largest group consists of elements that exhibit transport behaviour determined mostly by their affinity for humic substance (HS) colloids naturally present in the pore water of Boom Clay. This means that a large part of the nuclide speciation in the Boom Clay pore water consists of humic-associated species (either as true complexes or as colloidal associations). Since these species are generally less well sorbed/retained, they will travel faster than their dissolved/inorganic counterparts. The following subgroups are distinguished:

- a. Dissolved Organic Matter (DOM) itself is considered as a reference tracer and it is assumed that humic colloid-associated species have the same transport properties as DOM.
- b. Heavy metals,
- c. Trivalent lanthanides/actinides, and
- d. Tetravalent lanthanides/actinides and the pentavalent Pa.

However, there is currently not enough experimental support to provide different migration parameters for these subgroups; instead rather general migration parameters are proposed (based on limited set of key nuclides: Tc, Am are most studied).

The conceptual model for the NOM-facilitated transport of the fourth group is schematised in Figure 21. It consists of a two-species equilibrium model, in which two components per radionuclide are allowed to migrate: the mobile complex (RN-OM) and the "free inorganic" radionuclide species in solution ($RN_{inorg,liquid}$). Both components are described by the classical advection-diffusion-reaction equation with linear sorption. Both species can interact with the solid phase. It is assumed that this interaction in the case of ($RN_{inorg,liquid}$) is mainly due to sorption processes and can be described by a retardation factor (R_{RN}) that can be linked to batch sorption data. Should the concentration of $RN_{inorg,liquid}$ exceed the thermodynamic solubility limit of the controlling phase in Boom Clay conditions, the RN is also allowed to precipitate. With respect to RN-OM, the retardation factor (R_{RN-OM}) is considered as a lumped factor, accounting for both sorption and colloid filtration processes. Diffusive DOM transport is characterised by weak, but non-negligible retardation, with retardation factors R_{DOM} (determined mostly under advection conditions) ranging typically from ($>$)1-10.

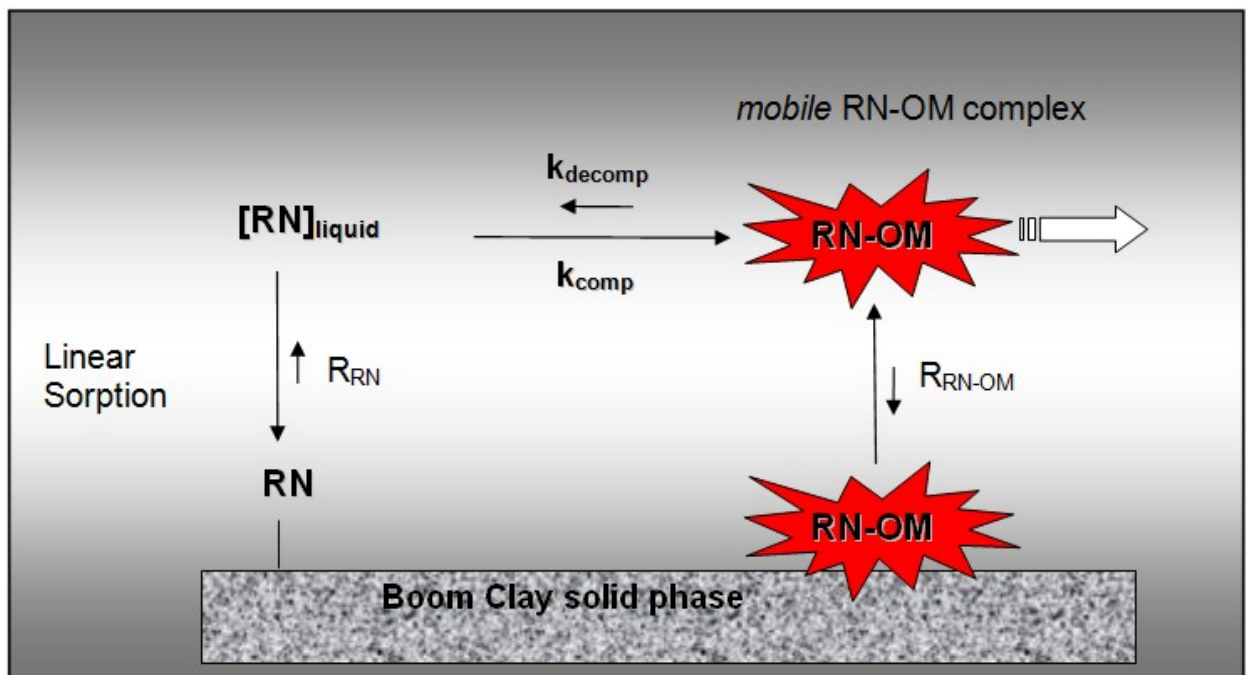


Figure 21: Conceptual model for DOM-linked transport of radionuclides.

The exchange of the radionuclide between $[RN_{inorg}]_{liquid}$ and the RN-OM complex is described by a complexation constant K_{comp} which is the ratio between the association (k_{comp})

and dissociation (k_{decomp}) kinetics. As the characteristic timescales of the complexation and decomplexation reactions are very small compared to the typical timescales in safety assessment calculations, the exact values of the kinetic rate constants do not have any impact on the results of the calculations. The interaction equations are further discussed in 5.2.2.

Far field solubility

Far field solubility limits are based on thermodynamic calculations in undisturbed Boom Clay conditions. The least stable mineral phase (i.e. kinetically favoured) is chosen as controlling the solubility, which yields the highest solubility limit. As time progresses, these unstable minerals will transform into more stable phases and solubility limits are expected to decrease. If available, solubility limits are backed up by experimental observations (U, Tc, Am). For RN that interact strongly with the organic matter in Boom Clay, the provided solubility limit is the predicted/calculated one in absence of organic ligands/complexes. In the transport calculations, the influence of organic complexation on the solubility of radionuclides is taken into account by calculating the equilibrium between organic and inorganic species, determined by the complexation constant and the DOM-concentration (Bruggeman *et al.*, 2010; Bruggeman *et al.*, 2011; Bruggeman *et al.* Integration report draft version, 2011; Salah and Wang, draft version, 2011) Substantial effort has been spent on the quality and consistency of the thermodynamic database (MOLDATA, Wang *et al.*, 2011).

As these solubility limits are only valid in undisturbed Boom Clay conditions, they are applied on the interface between the disturbed zone and the undisturbed zone. However, this interface is located approximately 4.5 m away from the waste, and at that distance the maximum radionuclide concentrations attained are several orders of magnitude lower than in the source. Therefore, only few radionuclides will ever become oversaturated in the far field and the contribution of this R3 process to long term safety is very small.

Other assumptions pertaining to the implementation of far field solubility are:

- Amorphous phases are also considered and even preferred to crystalline phases in the data selection process although the latter are thermodynamically more stable on the long-term. Solid solution and co-precipitation processes are not considered.
- The precipitation/dissolution of radionuclide bearing minerals is assumed to be an instantaneous process. Any impact due to precipitation/dissolution processes on the porous nature of the domain is not considered.
- The solubility of the least stable mineral phase is implemented as a fixed value (no time evolution) and are assumed to remain valid over the whole assessment timeframe.
- The concentrations of the most important stable isotopes in the waste (Se and Pd) are taken into account in calculating the effective solubility limit.
- The solubility limits of the different isotopes (e.g. uranium) is obtained from the product of the isotope fraction in the waste and the solubility limit of the element.

5.1.6 Dilution in aquifer systems

After the slow diffusive transport through the Boom Clay layer, in which a large fraction of the initially present radiological inventory will have decayed, only a small fraction of the radionuclides will enter the aquifer systems surrounding the Boom Clay. In these aquifer systems (the Neogene aquifer above and the Lower-Rupelian aquifer below Boom Clay), the radionuclides will become diluted and dispersed. Eventually, some may reach the biosphere, for instance through a water well or through draining rivers. As already mentioned in paragraph 3.3,

the Neogene aquifer is considered a far more important biosphere receptor than the Lower-Rupelian aquifer, and therefore the latter is not further discussed in the reference scenario.

The radionuclide travel times through the aquifers are much smaller than in the clay, although the spatial scale is larger. For non-retarded nuclides, travel times through the clay are expressed in tens of thousands of years, while the aquifer response time to a constant influx does not exceed a few thousand years. In fact, the advective transport in the aquifers is so much faster than the diffusion of nuclides through the Boom Clay that a quasi-steady aquifer model can be used. This unit flux approach consists of calibration of the hydrogeological model and performing a single transport simulation for a unit, constant injection rate source of a conservative tracer at the repository location, and monitoring the concentration evolution in the different geological layers. The actual concentrations of each nuclide in the groundwater and its fluxes into the rivers can then be obtained by multiplying the results for the unit flux simulation by the effective flux out of the Boom Clay for the considered nuclide and, if necessary, by correcting for the decay.

Such an approach is conservative, as it neglects the small buffer effect of the aquifer on nuclide release. Moreover, as the nuclides that are sorbed by the aquifer sands can be assumed to be the same as those that are also strongly sorbed by the Boom Clay, this quasi-steady approach seems reasonable even for retarded nuclides, because the assumption on the relative time scales of transport in clay and aquifers still holds.

To summarise, to take the "dispersion and dilution" role of the aquifers into account in the integrated performance assessment, the dilution of the radionuclide concentrations occurring in the aquifers are quantified by a set of dilution coefficients. These coefficients can be computed with realistic and detailed models for present conditions and a sufficiently characterised site. Furthermore, although the uncertainty on aquifer (and biosphere) evolution is considerable, the dilution coefficients are taken constant in time for the whole assessment timeframe. In other words, the evaluation of the *performance of the disposal system* focuses on the engineered and natural barriers, while downstream processes which are subject to more uncertainty, are treated in a stylised manner in ONDRAF/NIRAS safety assessment methodology (ONDRAF/NIRAS, 2009c). This approach is consistent with international safety assessment methodologies (NEA, 2004; NEA, 2012). Complementary assessments can be made, that take into account climate evolution into hotter or colder climate types, but these fall outside the scope of the reference case.

Considered water well

The considered water well is assumed to be drilled at a very unfavourable location in the Neogene aquifer. The filter of the well is assumed to be placed at the location of the highest concentrations in the hydrogeological model. In the deepest aquifer layer that still has a sufficiently high hydraulic conductivity, this location is somewhere between the downstream border of the repository and the principle draining river. It is also assumed that a relatively small amount of water (5000 m³/year) is pumped from the well. This has little effect on the groundwater flow and the pumped water is thus not diluted by less contaminated water being drawn in from overlying water bearing strata.

Dilution coefficient calculated for the Mol site

Calculations of radionuclide transport in the Neogene aquifer based on the unit flux approach were done by Hardy and Marivoet (2000). This solute transport model made use of the flow field calculated by Meyus *et al.* (2000) with a local model (the size of the model area was about 20

km × 8 km) for the Mol area in a study of flow and transport in the Neogene aquifer. The most notable improvement of the transport calculations done by Hardy and Marivoet (2000) in comparison with those done by Meyus *et al.* (2000) was an increase of the vertical discretisation to improve the representation of the transverse dispersion processes.

In the vertical direction the Neogene aquifer consists of five different sand layers. Figure 22 gives a schematic representation of the considered geological layers, their thickness and hydraulic conductivity for the local flow and transport model.

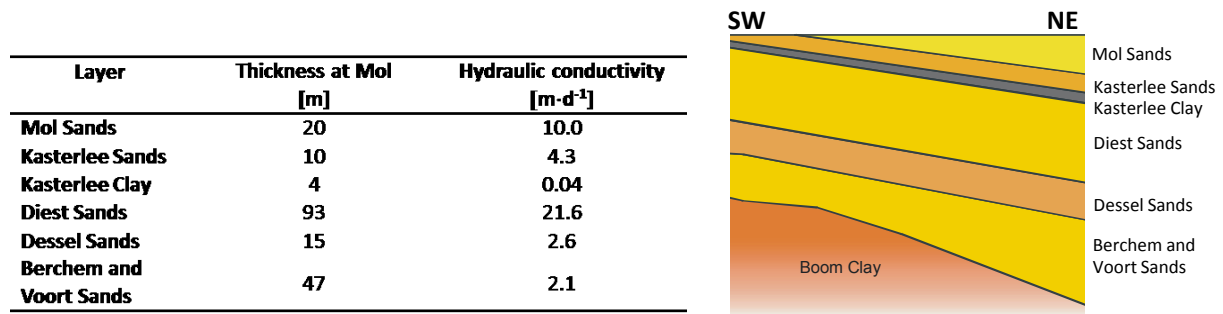


Figure 22: Schematic overview of the Neogene aquifer layers, their thickness and hydraulic conductivity as implemented in the hydrogeological model of the Mol site.

As explained above, the aquifer transport calculations are based on a quasi-steady state simulation. As a “unit” case, the steady transport through the Neogene of the long-lived and unretarded I-129 nuclide, considered here as a conservative tracer, was calculated for a 1 MBq/a flux out of the Boom Clay in the area above the repository. Concentration contours for this unit case are shown in Figure 23 to Figure 25 for different layers of the Neogene aquifer. The maximum concentration in the groundwater of each layer is reported in Table 13 and the fluxes into the rivers are presented in Table 14. The river sections can be identified using Figure 26.

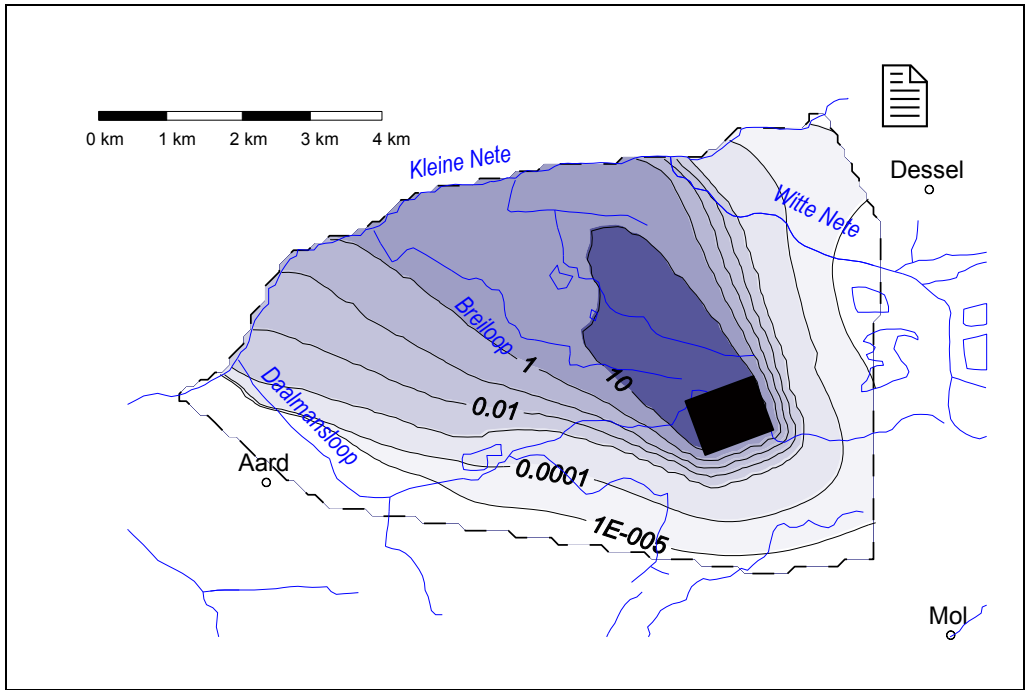


Figure 23: Radionuclide concentration (Bq/m^3) in the waters of the Berchem Sands for a 1 MBq/a flux out of the Boom Clay.

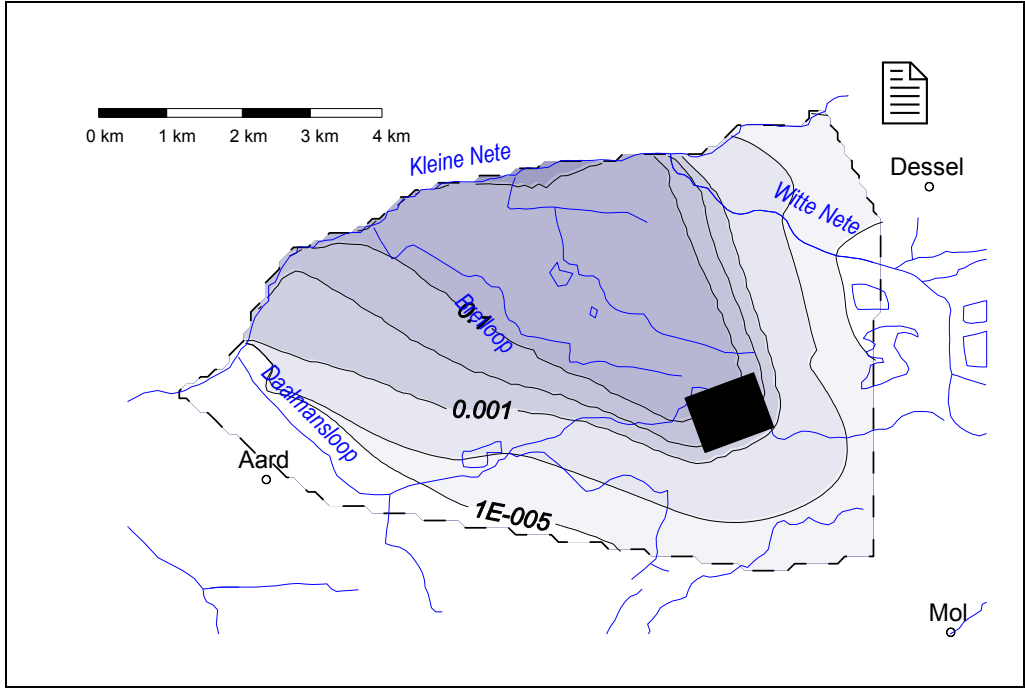


Figure 24: Radionuclide concentration (Bq/m^3) in the waters of the Diest Sands for a 1 MBq/a flux out of the Boom Clay.

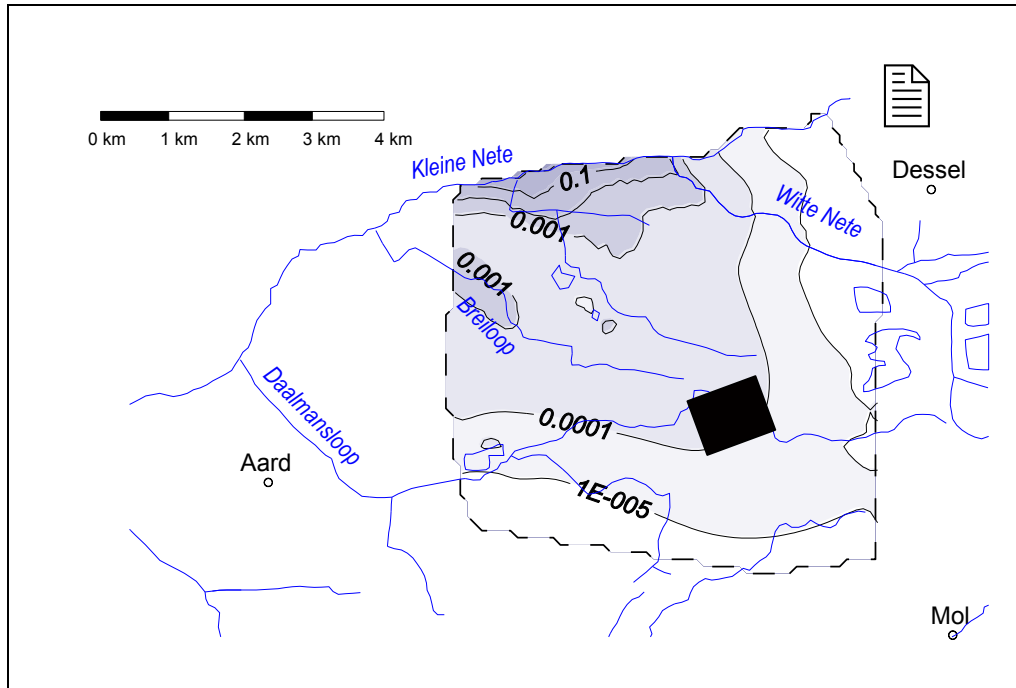


Figure 25: Radionuclide concentration (Bq/m^3) in the waters of the Mol Sands for a 1 MBq/a flux out of the Boom Clay.

As can be seen in Table 14, practically all the radionuclide particles ultimately reach the river Kleine Nete, either indirectly via the Witte Nete (river sections 2-3), or directly (river sections 4-7). For the dose calculations it is assumed that 100% of the flux released from the host clay layer into the Neogene aquifer enters into river section 3. This approach is conservative because the river flow (and thus the resulting dilution) is smaller in the upstream section 3 than in the more downstream sections 4, 5 and 6.

The most adverse location for a drinking water well in the deeper layers (Dessel, Berchem and Voort Sands) is above the downstream or North-northwest side of the repository. In the upper layers (Mol, Kasterlee and Diest Sands), the concentrations reach their maximum values near the Kleine Nete river. This means that the particle plume remains flat and only close to the river the plume goes (almost vertically) upwards towards the draining river. If a small well is considered, the radionuclide concentration of nuclides in the pumped water can conservatively be assumed to be at most equal to the maximum concentration in the groundwater.

Table 13: Maximum calculated concentrations in the groundwater for a 1 MBq/a flux out of the Boom Clay (adapted from Hardy and Marivoet (2000), Table 5.2.1).

Layer	Maximum concentration (Bq/m^3)
Mol Sands	2.25
Kasterlee Sands	2.71
Diest Sands	6.06
Dessel Sands	11.65
Berchem and Voort sands	89.81

Table 14: Calculated RN fluxes into the rivers for a 1 MBq/a flux out of the Boom Clay (adapted from Hardy and Marivoet (2000), Table 5.2.2). Note that the river section that receives the highest flux (section 3) is surprisingly still called “Witte Nete”.

Section	Location	Flux (Bq/a)	Percentage (%)
1	Desselse Nete	1732	0.2
2	Witte Nete	18945	2.3
3	Witte Nete	429903	51.3
4	Kleine Nete	83943	10.0
5	Kleine Nete	128825	15.4
6	Kleine Nete	145391	17.4
7	Kleine Nete	1981	0.2
8	Hooibeek	16978	2.0
9	Breilooop (north)	8372	1.0
10	Dalemansloop	1255	0.1
11	Breilooop	9	<0.1
12	Prinsenpark	<1	<0.1
13	Visvijver	187	<0.1
14	Zeggeloop	0	0.0
15	Kleine Nete	0	0.0
16	Witte Nete	0	0.0
17	Sand Pits	0	0.0

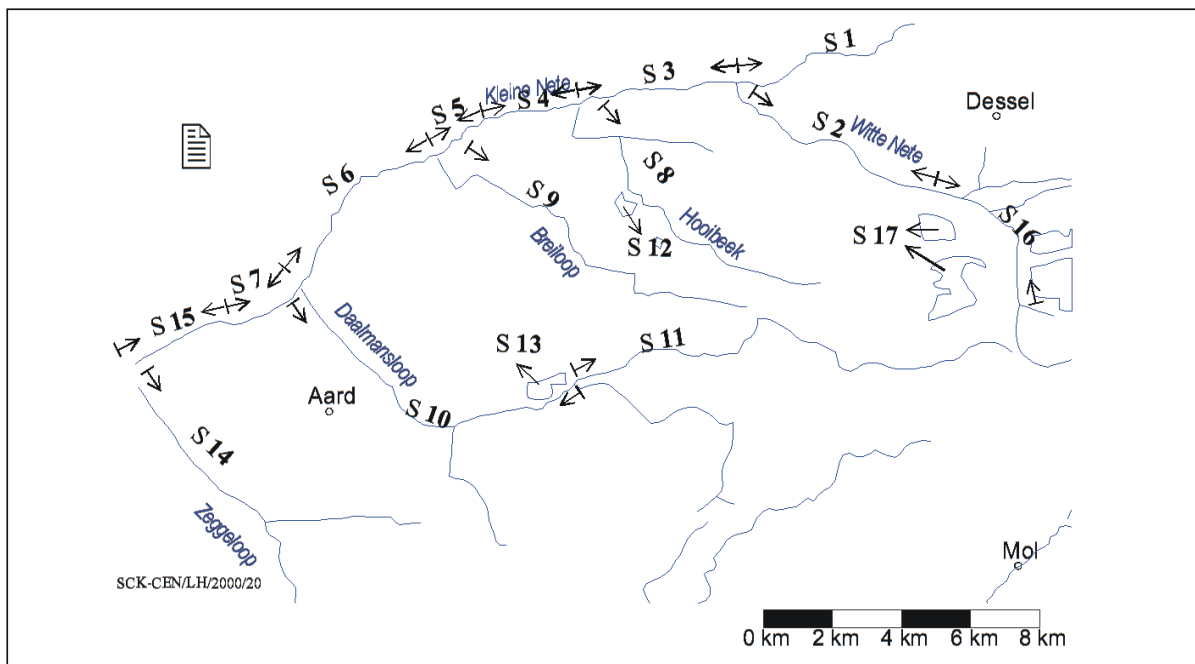


Figure 26: Identification of the river cross-sections (from Hardy and Marivoet, 2000)

Overall the highest concentrations are to be found in the lowest aquifer parts: Berchem and Voort Sands, and Dessel Sands (see Table 13). However, the hydraulic conductivity of these layers is relatively low. Although pumping in these layers is technically feasible to extract small volumes, there is reason to assume that it is very unlikely. Indeed, pumping in the above lying Diest Sands is much more likely, because it is less deep (hence cheaper), and has a 10 times higher yield. Therefore, a well in the Diest Sands with a maximum concentration of 6.06 Bq/m^3 for a unit flux of 1 MBq/a is selected as reference biosphere receptor. The corresponding dilution rate is then $165\,000 \text{ m}^3/\text{a}$.

5.1.7 Radionuclide transport in the biosphere

Biosphere modelling part of safety assessment consists of the interpretation of the transport of radionuclides released into the biosphere and their impact on human health. The biosphere models are steady state models, yielding biosphere conversion factors starting from a unit flux (river pathway) or unit concentration (well pathway) approach.

The following applications of water from the well and the river are considered:

- for the water well: water pumped from the well is used as drinking water, for irrigation of crop fields and pastures, and as drinking water for the cattle;
- for the river: groundwater drained by the river from the aquifer has to percolate through the river bed sediment layer where a number of radionuclides are sorbed on the sediments; the river water is first filtrated when it is used as drinking water; it is directly used for irrigation of crop fields and pastures, and as drinking water for the cattle; fishes live in the river and the river can be used for recreation (e.g. fishing).

All relevant processes and transfers of radionuclides considered in the biosphere model are given in Olyslaegers *et al.* (2009) and Sweeck *et al.* (2011). A scheme of the considered biosphere conceptual model is shown in Figure 27.

The biosphere model considers the following exposure pathways:

- ingestion of drinking water, food crops, milk, meat and eggs, and fish (the latter for the river pathway only);
- inhalation of resuspended dust and radon from crop fields;
- external irradiation of man on crop fields and river banks.

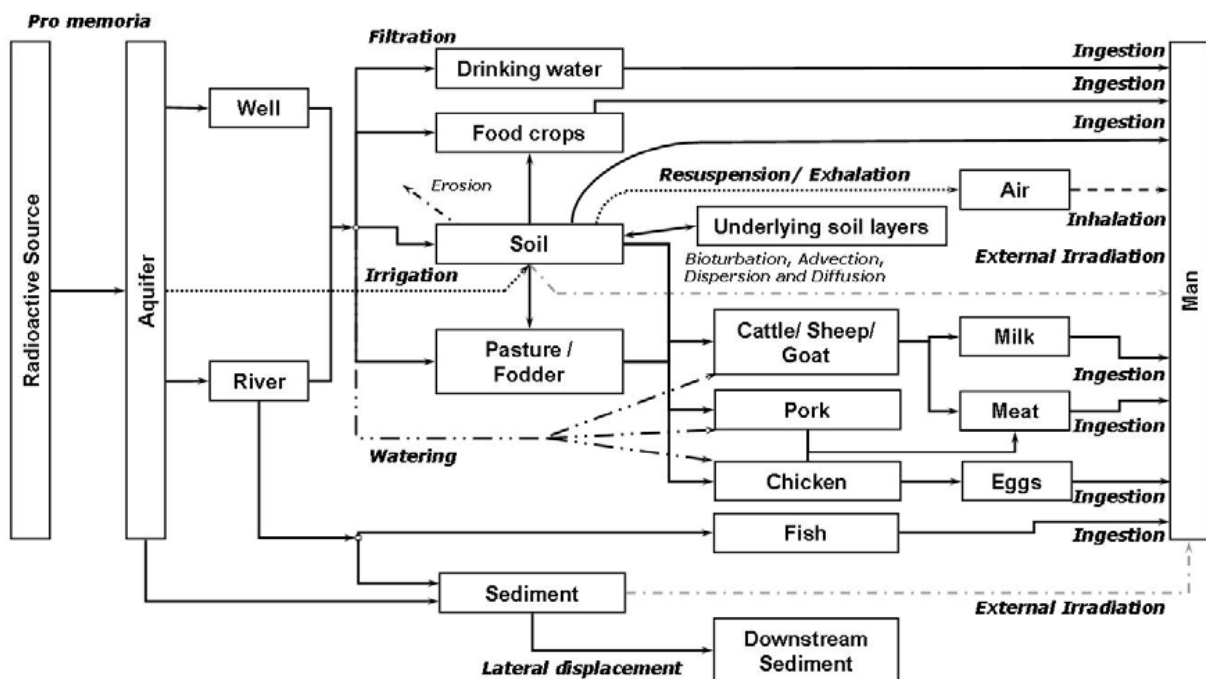


Figure 27: Conceptual model for biosphere assessment.

Age groups

ICRP publication 101 (2006) now recommends the use of three age categories for estimating annual dose to the representative person for prospective assessments. These categories are 0-5 years (infant), 6-15 years (child), and 16-70 years (adult). For practical implementation of this recommendation, dose coefficients and habit data for a 1-year-old infant, a 10-year-old child, and an adult are used to represent the three age categories, and corresponding biosphere conversion factors for well and river pathway are calculated.

5.2 Mathematical model

5.2.1 Domain and geometry

The near field and the Boom Clay are modelled together. As the radionuclide travel times through the aquifers are much smaller than in the clay, a quasi-steady aquifer model can be used (see section 5.1.6). This allows uncoupling of diffusive migration through near field and clay on the one hand and advective transport in the aquifers on the other hand. The aquifer is represented in the reference model through a zero concentration (infinite dilution) boundary condition, thereby slightly overestimating the radionuclide fluxes across that boundary.

Because the thickness of the Boom Clay layer is significantly smaller than the length of the disposal galleries (possibly up to 1000 m) and in the absence of horizontal advection (*i.e.* no preferential pathways along the galleries and shaft), the real world three-dimensional geometry can be simplified into 2D cross-sections perpendicular to the galleries. As the disposal galleries are identical, the radionuclide migration effectively needs to be computed for a single gallery, throughout the enclosing rectangular clay volume (conservative hypothesis). In the absence of significant advective transport through the clay layer, the model can be further reduced to a fourth of its original size because of horizontal and vertical symmetry lines crossing the gallery axis (Figure 28). The mathematical and numerical models are further discussed in paragraph 5.2.

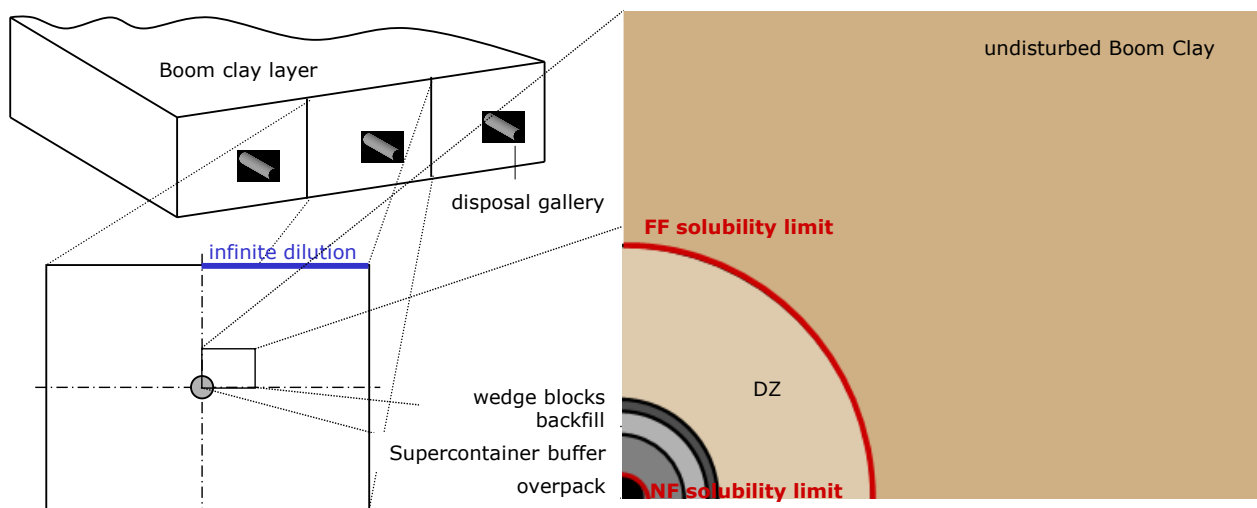


Figure 28: Model dimensionality reduction and near field geometry.

5.2.2 Governing transport equations

The conservation equation for convective-dispersive-reactive transport with linear reversible sorption in saturated porous media is (Fetter, 1999)

$$(\eta + \rho_b K_d) \frac{\partial c}{\partial t} - \nabla \cdot \left[\eta(D + D_p I) \nabla c + u_{Darcy} c \right] = -\lambda(\eta + \rho_b K_d)c + r + S \quad (1)$$

where c is the concentration of a given nuclide in the pore water, η is the porosity, ρ_b is the bulk density, K_d is the distribution coefficient, D is the hydrodynamic dispersion tensor, D_p is the pore diffusion coefficient, I is the identity matrix, u_{Darcy} is the Darcy velocity, λ is the decay rate, r is the reaction rate (precipitation/dissolution), S is the solute source which in this case is the release of radionuclides from the waste matrix.

As explained in section 5.1.4, convective and dispersive transport can be neglected. The flux of nuclides through a macroscopic section of porous media can be computed as

$$F_{por.media} = -\eta D_p \frac{\partial c}{\partial x} \quad (2)$$

The transport equation can be simplified by dividing it by η and the retardation factor R :

$$\frac{\partial c}{\partial t} - \nabla \cdot \left[\frac{D_p}{R} \nabla c \right] = -\lambda c + r' + S' \quad (3)$$

with

$$R = 1 + \frac{\rho_b K_d}{\eta} \quad (4)$$

5.2.3 Transport equations of actinide decay chains

For decay chains, a system of equations similar to equation (3) has to be solved, where the source term of the transport equation for a given radionuclide corresponds to the decay term of the transport equation for the parent nuclide.

The transport equation for the parent radionuclide is:

$$\frac{\partial c_0}{\partial t} = \nabla \cdot \left(\frac{D_{p,0}}{R_0} \nabla c_0 \right) - \lambda_0 c_0 + r_0 + S_0 \quad (5)$$

If concentration is expressed in mol/l, the transport equation for the first daughter radionuclide is:

$$\frac{\partial c_1}{\partial t} = \nabla \cdot \left(\frac{D_{p,1}}{R_1} \nabla c_1 \right) - \lambda_1 c_1 + \lambda_0 \frac{R_0}{R_1} c_0 + r_1 + S_1 \quad (6)$$

and for the second daughter radionuclide:

$$\frac{\partial c_2}{\partial t} = \nabla \cdot \left(\frac{D_{p,2}}{R_2} \nabla c_2 \right) - \lambda_2 c_2 + \lambda_1 \frac{R_1}{R_2} c_1 + r_2 + S_2 \quad (7)$$

and so on.

If (activity) concentration is expressed in Bq/m³, equation for the first daughter radionuclide is:

$$\frac{\partial c_1}{\partial t} = \nabla \cdot \left(\frac{D_{p,1}}{R_1} \nabla c_1 \right) - \lambda_1 \left(c_1 - \frac{R_0}{R_1} c_0 \right) + r_1 + S_1 \quad (8)$$

and for the second daughter radionuclide:

$$\frac{\partial c_2}{\partial t} = \nabla \cdot \left(\frac{D_{p,2}}{R_2} \nabla c_2 \right) - \lambda_2 \left(c_2 - \frac{R_1}{R_2} c_1 \right) + r_2 + S_2 \quad (9)$$

and so on.

5.2.4 Reaction rate (precipitation/dissolution)

The precipitation/dissolution reaction is assumed to be instantaneous. The first implication is that both dissolution and precipitation rate constants are equal. Assuming zeroth order rate reaction, the reaction rate r for instantaneous precipitation/dissolution can be expressed as:

$$r = \begin{cases} k_s(c_{sat} - c) & \text{if } c < c_{sat} \text{ and } c_p > 0 \\ -k_s(c - c_{sat}) & \text{if } c > c_{sat}. \end{cases} \quad (10)$$

where k_s is the precipitation/dissolution rate constant, c_{sat} the solubility limit and c_p the concentration of the precipitate. As the precipitation/dissolution is assumed to be instantaneous, k_s merely serves as a tuning parameter (usually a high value) in order to limit the liquid concentration at the maximal solubility value. The first expression of equation (10) represents control of dissolution rate and the second expression represents control of precipitation rate.

5.2.5 Dissolved Organic Matter (DOM) facilitated transport

Transition metals, actinides and lanthanides are known to form strong complexes with humic substances. The conceptual model for this DOM-facilitated transport is explained and schematised Figure 21.

In this model, two components per radionuclide are allowed to migrate: the dominant (as revealed by the speciation calculations) dissolved inorganic species under Boom Clay conditions (typically a neutral hydrolysed species or a negatively charged complex with carbonate and/or hydroxy ligands) and the species (*i.e.* radionuclide) associated with a humic substance colloid.

Radionuclides (RN) in solution will either be described as a mobile RN-OM complex or “free inorganic” radionuclide species in solution ($[RN]_{inorg}$). Both components are described by the classical advection-diffusion-reaction with linear sorption equation. The transport of the RN-OM mobile complex is described by:

$$(\eta + \rho_b K_{d,RNOM}) \frac{\partial(c_{RNOM})}{\partial t} - \nabla \cdot [\eta D_{p,RNOM} \nabla c_{RNOM} + u_{Darcy} c_{RNOM}] = -\lambda(\eta + \rho_b K_{d,RNOM}) c_{RNOM} + \eta Q_{sol-OM} \quad (11)$$

The transport of the free RN-species in solution is described by:

$$(\eta + \rho_b K_{d,RN}) \frac{\partial(c_{RN})}{\partial t} - \nabla \cdot [\eta D_{p,RN} \nabla c_{RN} + u_{Darcy} c_{RN}] = -\lambda(\eta + \rho_b K_{d,RN}) c_{RN} - \eta Q_{sol-OM} \quad (12)$$

where c_{RN} , c_{RNOM} , c_{OM} are the concentrations of free inorganic radionuclide species in solution, concentration of the mobile RN-OM complex and the concentration of the mobile OM, respectively. $D_{p,RNOM}$ and $D_{p,RN}$ are the pore diffusion coefficients (D_p) of the RN complexed to the mobile OM and of the free inorganic RN species in solution, respectively.

The exchange of the radionuclide between $[RN_{inorg}]_{liquid}$ and the RN-OM complex is described by a complexation constant which is the ratio between the association and dissociation kinetics. The mass transfer (Q_{sol-OM}) of the RN between the OM complexed form and the “free” RN in solution is given by:

$$Q_{sol-OM} = k_{comp} c_{RN} c_{OM} - k_{decomp} c_{RNOM} \quad (13)$$

$$[RN_{inorg}] + [OM] \xrightleftharpoons[k_{decomp}]{k_{comp}} [RN-OM] \text{ and } K_{RN-OM} = \frac{k_{comp}}{k_{decomp}} = \frac{c_{RNOM}}{c_{RN} \cdot c_{OM}} \quad (14)$$

where k_{comp} and k_{decomp} are the kinetic rate constants for the RN-OM complexation (association) and decomplexation (dissociation) reactions, respectively; and K_{RNOM} is the equilibrium constant. As characteristic timescales of the complexation and decomplexation reactions are very small compared to typical timescales used in PA calculations, the exact values of the kinetic rate constants do not have any impact on the results. The kinetic dissociation constant, k_{decomp} , is of the order of 10^{-7} s^{-1} .

Both species can interact with the solid phase. It is assumed that this interaction in the case of $[RN_{inorg}]_{liquid}$ is mainly due to sorption processes and can be described by a retardation factor (R_{RN}) that can be linked to batch sorption data. Most frequently, the dissolved species is characterised by a very strong retardation, as shown through batch experiments. Typically, the retardation factor R_{RN} is in the range of 10^3 - 10^5 . $K_{d,RNOM}$ and $K_{d,RN}$ are the sorption distribution coefficients (K_d) for the RN complexed to the mobile OM and for the free inorganic RN species in solution, respectively. They are related to the retardation factors R_{RNOM} and R_{RN} by equation (4).

R_{RN-OM} is considered as a lumped factor, accounting for both sorption and colloid filtration processes. Diffusive DOM transport is characterised by weak, but non-negligible retardation, with R_{DOM} ranging typically from 1 to 10 (determined mostly under advection conditions).

5.2.6 Calculation of safety and performance indicators

As calculation endpoints of the integrated safety assessment model, a set of safety and performance indicators is selected, as explained in paragraph 4.3. The calculation procedure is detailed below, using the following nomenclature (Marivoet *et al.*, 2010):

- **Radionuclides** are numbered by n .
- The **ingestion dose coefficient** D_n is the dose caused by ingestion of radionuclide n . (Sv per ingested Bq). The ingestion dose coefficients of ICRP publication 72 (1996) for adults
- The **biosphere dose conversion factor** B_n is the annual dose to a representative person caused by a unit concentration of radionuclide n in the biosphere water. Its unit is in $[(\text{Sv/a})/(\text{Bq/m}^3)]$ for the well pathway and $[(\text{Sv/a})/(\text{Bq/a})]$ for the river pathway.
- d_{well} is the **dilution factor** (a/m^3) for the well pathway, defined as the inverse of the dilution rate (see 5.1.6)
- c_n is the **activity concentration** (Bq/m^3) of radionuclide n in the biosphere water.
- $a_{n,i}$ is the **activity** (Bq) of radionuclide n in compartment i .
- $s_{n,i}$ is the **activity flux** (Bq/a) of radionuclide n from compartment i .
- $a_{n,in}$ is the **initial activity inventory** (Bq) of radionuclide n that has the potential to be released.

SI-1 Annual effective dose (Sv/a)

The individual dose rate represents the annual effective dose to an average member of the group of the most exposed individuals.

Calculation for well pathway:
$$\sum_n s_{n,host\ formation} d_{\text{well}} B_{n,\text{well}}$$

Calculation for river pathway:
$$\sum_n s_{n,host\ formation} B_{n,\text{river}}$$

SI-2. Radiotoxicity concentration in aquifer water (Sv/m³)

The indicator represents the radiotoxicity of the radionuclides in 1 m³ of aquifer water.

Calculation:
$$\sum_n s_{n,host\ formation} d_{\text{well}} D_n$$

SI-3. Radiotoxicity flux released from the host formation (Sv/a)

The indicator represents the radiotoxicity of the radionuclides released from the host formation to the biosphere in a year.

Calculation:
$$\sum_n s_{n,host\ formation} D_n$$

PI-1 Activity in compartments (Bq)

The indicator represents nuclide-specific activities as well as the total activities summed over all radionuclides in the compartments.

Calculation:
$$a_{n,i}; \sum_n a_{n,i}$$

PI-2 Radiotoxicity in compartments (Sv)

The indicator represents nuclide-specific radiotoxicity as well as the total radiotoxicity in the compartments.

Calculation:
$$a_{n,i} D_n; \sum_n a_{n,i} D_n$$

PI-3 Integrated activity flux from compartments (Bq)

The indicator represents the cumulated activity flux from compartment i to $i+1$ for single radionuclides as well as summed over all nuclides.

$$\text{Calculation: } \int_0^t s_{n,i}(\tau) d\tau; \sum_n \left(\int_0^t s_{n,i}(\tau) d\tau \right)$$

PI-4 Performance indicators based on safety functions

Performance indicators can be defined for each of the safety functions identified in the safety strategy (ONDRAF/NIRAS, 2009a) to contribute to the confinement of the radionuclides in the repository system in the case of the reference scenario. The proposed set of indicators is based on "released fractions", which are defined as follows:

$$\text{released fraction} = \text{activity}_{\text{out}} / \text{activity}_{\text{in}}$$

The calculation procedure for this set of indicators is the following:

- containment (C):
 $PI_C = \text{activity}_{\text{in WP}(T1)} / \text{activity}_{\text{in WP}(T0)}$
with: $\text{activity}_{\text{in WP}(T0)}$: initial activity in waste package (T0= time of disposal)
 $\text{activity}_{\text{in WP}(T1)}$: activity in waste package at time of overpack failure (T1)
- limitation of release (R1):
 $PI_{R1}(t) = \text{activity}_{\text{out WP}(t)} / \text{activity}_{T1}$
with: $\text{activity}_{\text{out WP}}$: time-integrated (up to time t) activity flux released from waste package
- retardation due to migration through buffer and host formation (R3):
 $PI_{R3}(t) = \text{activity}_{\text{out HF}(t)} / \text{activity}_{\text{out WP}(t)}$
with: $\text{activity}_{\text{out HF}}$: time-integrated activity flux released from host formation

The product of the 3 indicators defined above gives an indication of the performance of the integrated repository system (IRS):

$$PI_{IRS}(t) = PI_C \times PI_{R1}(t) \times PI_{R3}(t) = \text{activity}_{\text{out HF}(t)} / \text{activity}_{T0}$$

6 Iterations of the reference case

This chapter shortly describes the previous steps of the preparatory safety assessments (cf. ONDRAF/NIRAS, 2009c).

Within SFC1, an initial version of the reference case (see Figure 29) has been defined in December 2009 based on knowledge from the previous formal safety assessment and adapted to the new repository concept of ONDRAF/NIRAS.

Then, an iterative refinement of the working version of the reference case has taken place (version 2 and 3; see Figure 29), based on exploratory calculations and identification of potentially safety-relevant uncertainties. A central issue is the data selection process, *i.e.* the selection of the source and expert ranges (see section 1.3) to be used in the safety assessments. The sensitivity of the safety assessments to the identified uncertainties was assessed by means of scoping calculations (*e.g.* uncertainty on expert or source range, or some types of model uncertainty) and supporting calculations (phenomenological uncertainty).

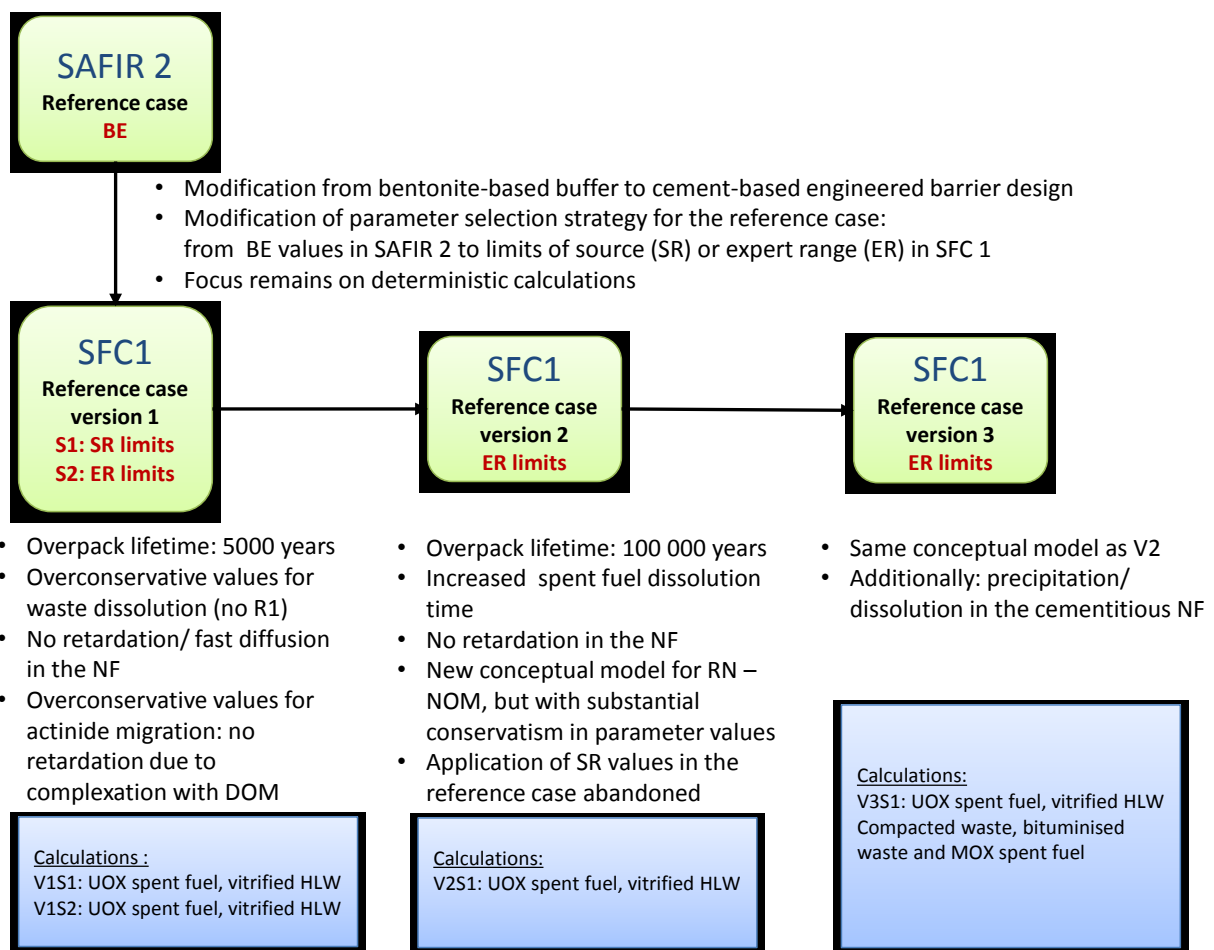


Figure 29: Versioning of the reference case.

6.1 Version 1

The initial working version of the reference case was based on the approach and results of the previous formal safety assessments reported in the SAFIR 2 report (ONDRAF/NIRAS, 2001). The repository concept at that time was based on a long steel disposal tube in the centre of the gallery. In this disposal tube, the waste, packed in a stainless steel overpack, would be inserted and the remaining space between the tube and gallery lining would be backfilled with bentonite blocks. In 2004, ONDRAF/NIRAS drastically changed its disposal concept for category C waste by choosing the supercontainer concept based on a carbon-steel overpack surrounded by a Ordinary Portland Cement (OPC)-based buffer. Also for category B waste, the new reference concept (monolith) involves a thick-walled concrete container. As a consequence, the repository near field drastically changed compared to the previous formal assessment. A number of potential safety-relevant features of the new concept were not accounted for in the initial working version of the reference case. The near field geochemistry of the supercontainer concept, optimised to support the containment (C) safety function, reflected on substantial uncertainties pertinent to the radionuclide releases from the waste matrices (R1). Moreover, as clay and cementitious materials have very contrasted chemistries that will interact, the contact between the Boom Clay and the cement-based repository components might lead to a degradation of both types of material, and the formation of a near field and a geochemical disturbed zone for which the transient chemical conditions are difficult to characterise. For both the near field and the disturbed zone very conservative transport properties were used in the initial version of the reference case. As solubility limits had been determined in equilibrium with Boom Clay geochemistry, precipitation/dissolution reactions could only be applied outside this disturbed zone.

For the clay transport model experimental results obtained in the period 2000-2008 indicated that the transport of several radionuclides is strongly influenced by their interaction with dissolved organic matter that is naturally occurring in the Boom Clay. As a first approach, it was proposed to use the migration parameters of mobile natural organic matter (NOM) without retardation for modelling the migration of radionuclides interacting with organic matter.

Scoping calculations were performed for vitrified high-level waste and UOX spent fuel with limiting values of both source (Govaerts et al., 2012a) and expert ranges (Govaerts et al., 2012b) of the safety parameters (these data were taken from spreadsheet SFC1-data-091204-V1.3.xls in the Vignette Knowledge Management system of ONDRAF/NIRAS). The first version was intentionally based on overconservative hypothesis in order to reassess the ONDRAF/NIRAS R&D program and to set new priorities to SFC1.

An analysis of the results obtained for Version 1 of the reference case led to drawing the following conclusions and recommendations for the next steps of the preparatory safety assessments:

1. Due to the use of an oversimplified conceptual model and very conservative migration parameters, all radionuclides which have possible interactions with NOM are modelled as diffusing without retardation. Amongst these radionuclides, the actinides are the main contributors to the total dose rate. An alternative conceptual model and/or more realistic model parameters are needed for modelling the transport of radionuclides interacting with NOM.

2. Various safety relevant features of the engineered barrier are not considered:
 - A very short overpack lifetime (5000 years) was used corresponding to the design requirement following the safety concept, because the experimental dataset in relevant repository conditions was not yet well developed.
 - After overpack failure, all waste matrices are considered to dissolve almost instantaneously due to the use of conservative dissolution rates. This is related to the choice of a new barrier concept, imposing highly alkaline and therefore completely different geochemical conditions in the vicinity of the waste compared to the bentonite concept in SAFIR 2. Experimental programmes covering this concept change were still in an embryonic stage at the beginning of the preparatory safety assessment phase, and the corresponding uncertainty was reflected in the conservatism of the waste dissolution parameters.
 - Fast diffusion (corresponding to diffusion in pure water) and no sorption are assumed in the first five meters (consisting of 2 m of concrete of buffer, backfill and liner and 3 m of the damaged zone of the clay formation) around the waste matrix.
 - No precipitation/dissolution occurs in the waste package or in the first 3 metres of the clay; precipitation is only considered in the undisturbed clay. The dilution at this point, in combination with the use of very conservative solubility limits, means that in the transport simulations most of the radionuclides will not precipitate.

3. There are (possibly) some overestimations in the inventory:
 - Most of the activation products in the inventory are overestimated by using the maximal allowable tolerances of the impurities in the alloys.
 - Nb is specifically added in the composition of the new M5/ZIRLO cladding alloys (with higher corrosion resistance allowing for higher burn-ups as major objective) of the spent fuel assemblies. Practically, only part of the Belgian assemblies is clad with M5/ZIRLO type (the oldest ones are not). However, as the exact fraction of assemblies with the new zirconium alloy was not known, it was assumed that all the claddings are made of this new zirconium alloy. As the old Zircaloy-4 has a Nb impurity content of typically 0.02 wt%, while the new cladding type (in Belgian reactors) contains typically 1.2 wt% Nb, the used inventory obviously overestimated the Nb-94 production (Danièle Boulanger, personal communication).

4. By using a clay barrier thickness of 40 m in the two-dimensional model, the disturbed zones are already implicitly accounted for. So, by explicitly assuming no retardation and fast diffusion in the first 3 meter of the clay domain, the effect of the DZ is included twice in the calculations.

6.2 Version 2

The following sections present the refinements implemented in Version 2 of the reference case.

6.2.1 *NOM-linked radionuclide transport*

A new conceptual model was developed to describe the transport of radionuclides that can form complexes with natural organic matter (see section 5.2.5). This model involves a number of

additional parameters, for which source and experts ranges needed to be selected. All radionuclides in this group are assumed to migrate similarly.

6.2.2 *Engineered containment*

The containment safety function heavily relies on the absence of localized corrosion phenomena. As explained in sections 4.4.3 and 5.1.2, the influx of corrosion-aggressive species that are formed in the EDZ or naturally present in Boom Clay, may induce localized corrosion. Supporting calculations showed that they will not reach the overpack in concentrations that exceed the threshold for inducing localized corrosion (Govaerts and Weetjens, 2010). Although there remains some uncertainty on the occurrence of localised corrosion processes in supercontainer conditions, the confidence in the concept of uniform corrosion, in line with the safety strategy, has increased. The deterministic nature of the uniform corrosion process allows to estimate the overpack lifetime by combining the estimated corrosion rate with a minimum thickness of the overpack for mechanical resistance. This has led to a revision of the containment lifetime: instead of a containment lifetime of 5000 years, as applied in Version 1 of the reference case (this value had been chosen rather arbitrarily based on the design requirement), it is now estimated to be 100 000 years. The longer containment period has also consequences for the spent fuel matrix dissolution rate (R1).

6.2.3 *Spent fuel matrix dissolution*

After 100 000 years the alpha activity in the spent fuel is more than one order of magnitude lower than it is after 5000 years. As a consequence, the spent fuel matrix conversion due to local oxidising conditions caused by the alpha activity is negligible. Additionally, supporting calculations assessing the hydrogen concentration in the vicinity of the waste showed that the hydrogen concentration levels sufficient to suppress oxidative dissolution are attained very soon and might persist for hundreds of thousands of years.

Both arguments strengthened the confidence that the relevant spent fuel matrix dissolution mechanism is non-oxidative dissolution, and therefore significantly longer spent fuel matrix lifetimes can be expected. For Version 2 the spent fuel matrix lifetime was taken equal to 350 000 years.

6.2.4 *Other refinements*

The results obtained in the SELFRAC and TIMODAZ projects showed that the diffusion coefficient in the Disturbed Zone can be taken equal to the one in undisturbed clay (Yu *et al.*, 2011).

On the basis of information on the cladding materials of the fuels used in the Belgian nuclear power plants obtained from SYNATOM, the Nb-94 inventory of the spent fuel (and of the CSD-C waste) was decreased with a factor 3.3.

Scoping calculations have been performed for spent UOX fuel and vitrified HLW using expert ranges (data taken from SFC1-data-110211-v1.12.xls on the Vignette Knowledge Management system of ONDRAF/NIRAS) for the model parameter values (Govaerts *et al.*, 2012c).

The results obtained for Version 2 of the reference case still suffer from over-conservatism. Especially the correlation between parameters and the effect of combination of uncertainty in different model parameters lead to an unrealistic over-conservative global system description.

6.3 Version 3

It was assumed that precipitation/dissolution reactions take place in the primary waste canister. As the waste package will be subjected to the highly alkaline conditions caused by the concrete pore water of the various cement-based repository components, solubility limits applicable in a concrete environment are used. The data selection was based on the available knowledge from the category A disposal programme, where for most radionuclides minima, best estimates and maxima of the solubility were derived in oxidising and reducing conditions for the four concrete degradation states. For Version 3, the solubility data were selected conservatively as the maximum value of the first three states, including the 95% confidence level, with the exception of uranium (see remark on p. 62).

Scoping calculations were performed for vitrified HLW and spent UOX fuel (Govaerts *et al.*, 2012d), spent MOX fuel (Yu and Weetjens, to be published) and CSD-C waste (Weetjens and Govaerts, to be published) using data from SFC1-data-110211-v1.13.xls on the Vignette Knowledge Management system of ONDRAF/NIRAS.

The main conclusions that could be drawn from the results of the Version 3 calculations are:

1. The results of the Version 3 migration model for radionuclides that can form complexes with organic matter are still over-conservative. It is necessary to consider correlation between model parameters to avoid an unrealistic description of the migration behaviour of RN-NOM complexes at repository scale
2. In the case of category B disposal the near field components do not provide a significant contribution to the confinement of the radionuclides: no containment phase, negligible matrix lifetimes. However, category B waste contains non-negligible activities of relatively long-lived activation products such as C-14 ($T_{1/2} = 5700$ y) and Nb-94 ($T_{1/2} = 20\ 000$ y). These radionuclides can give doses that are of the same order of magnitude as the doses due fission products and actinides in the case of spent fuel or vitrified HLW disposal. Moreover, these peak doses occur at much earlier times.

6.4 Version 4

This version will take into account the conclusions of the uncertainty workshop, held in October 2011 in Mol, Belgium, and will include a major revision of the parameter dataset.

7 References

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Annex: Selection of radionuclides to be considered in the reference case

A1 Fission and activation products

The radionuclide inventories of the various existing and anticipated waste forms provided by ONDRAF/NIRAS contain a large number of radionuclides. The activity of radionuclides decreases with time because of radioactive decay. The slow solute migration through the Boom Clay layer makes that several of them will have decayed to negligible activities when reaching the clay-aquifer interface. Therefore, the list of radionuclides considered for safety calculations is based on a screening criterion that compares radionuclide half-life with their diffusive transport time through the host formation. This resulted in a shortlist of 12 relevant radionuclides (see Table 15). The radionuclide Sm-147, identified in SAFIR-2 as potentially safety-relevant, is omitted since its extremely long half-life (1×10^{11} years) makes it hardly radioactive.

In SAFIR-2 (ONDRAF/NIRAS, 2001) the following criterion was used:

Radionuclide is screened in if $T_{1/2} > F \times T_{diff}$, with

- diffusion time $T_{diff} = L^2 / (2 \times D_{app})$, where L is the distance between the repository and the clay-aquifer boundary (m), and D_{app} is the apparent diffusion coefficient (m^2/s)
- the coefficient F derived as follows:
 - 1) for the SAFIR-2 parameters ($L = 40$ m; $D_{app} = 2 \times 10^{-10} m^2/s = 6.312 \times 10^{-3} m^2/a$) the diffusion time of a conservative tracer T_{diff} was 126 750 years
 - 2) the breakthrough time was estimated on the basis of log-log diagrams to be about 5000 years, thus $T_{bt} = 0.04 \times T_{diff}$. Furthermore, to be very conservative, a safety factor 2 was introduced: this gives $T_{bt} = 0.02 \times T_{diff}$;
 - 3) after 30 half-lives, radionuclide activity is reduced by a factor 10^9 .

Combination of the three above elements led to $F = 0.00067$.

For the safety assessment calculations of SFC1, which include scoping calculations in the framework of the preparatory safety assessment (PSA) and the formal safety assessment (FSA) calculations, the same criterion is proposed with a revision of the F factor:

- 1) using the following parameters of the indicators report (Marivoet *et al.*, 2010): $L = 38.2$ m; $D_{app} = 1.4 \times 10^{-10} m^2/s = 4.418 \times 10^{-3} m^2/a$, the corresponding T_{diff} is 165 000 years for an unretarded radionuclide;
- 2) the breakthrough time can be defined as the time after which the flux released from the clay formation is only a fraction (0.1 or 1%) of its peak value for an impulse injection of a conservative tracer. From Figure 30, a breakthrough time of 7700 years (0.1%) or 10 200 years (1%) was derived. This corresponds to $T_{bt} = 0.047 \times T_{diff}$ (0.1%) or $T_{bt} = 0.062 \times T_{diff}$ (1%) respectively;
- 3) after 20 half-lives, radionuclide activity is reduced by a factor 10^6 .

Combining breakthrough time with radioactive decay gives the screening criterion $T_{1/2} > 0.0031 \times T_{diff}$ (1%) or $T_{1/2} > 0.0023 \times T_{diff}$ (0.1%). After conservative rounding, the following generalized selection criterion was fixed: $T_{1/2} > 0.001 \times T_{diff}$.

On the basis of this criterion, the following fission and activation products are screened in (Table 15):

Table 15 Fission and activation products relevant for performance assessment. The values for apparent diffusion coefficient are indicative best estimate values, with a simplified organic matter complexation model based on a lumped K_d approach.

Radionuclide	Half-life (y)	D_{app} (m ² /s)
C-14	5.70×10^3	6.00×10^{-11}
Cl-36	3.01×10^5	1.40×10^{-10}
Ca-41	1.03×10^5	7.90×10^{-12}
Ni-59	7.60×10^4	7.90×10^{-12}
Se-79	3.56×10^5	1.20×10^{-10}
Zr-93	1.53×10^6	2.30×10^{-10}
Nb-94	2.00×10^4	6.00×10^{-11}
Tc-99	2.14×10^5	2.30×10^{-10}
Pd-107	6.50×10^6	2.30×10^{-10}
Sn-126	2.30×10^5	2.30×10^{-10}
I-129	1.61×10^7	2.30×10^{-10}
Cs-135	2.30×10^6	1.40×10^{-13}

This list corresponds to the inventory data provided by ONDRAF/NIRAS for the long-lived fission and activation products (see also Figure A-2).

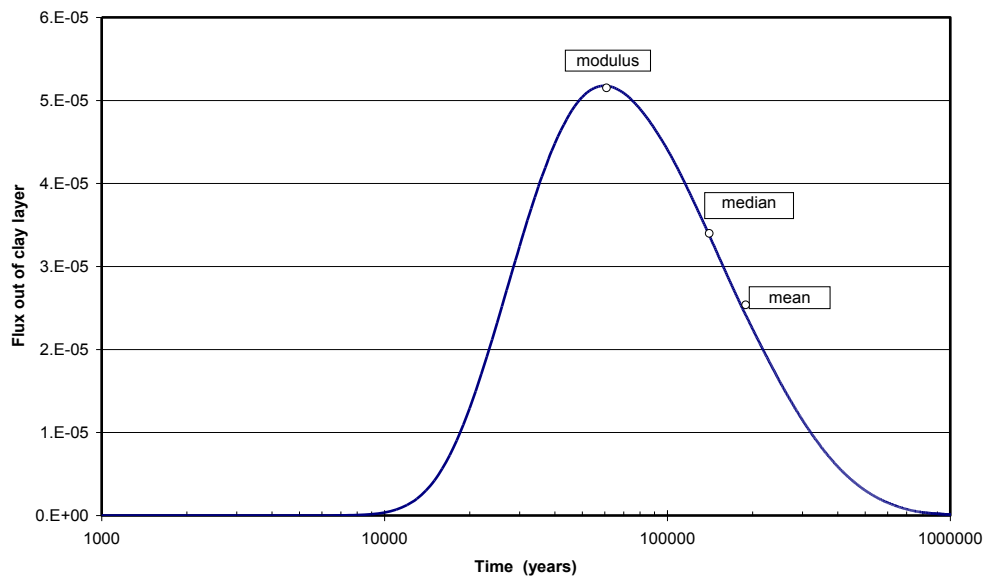


Figure 30: Evolution of the flux out of the clay layer for a pulse source (from Marivoet et al., 2010).

Figure 31 shows the screening criterion in a visual manner.

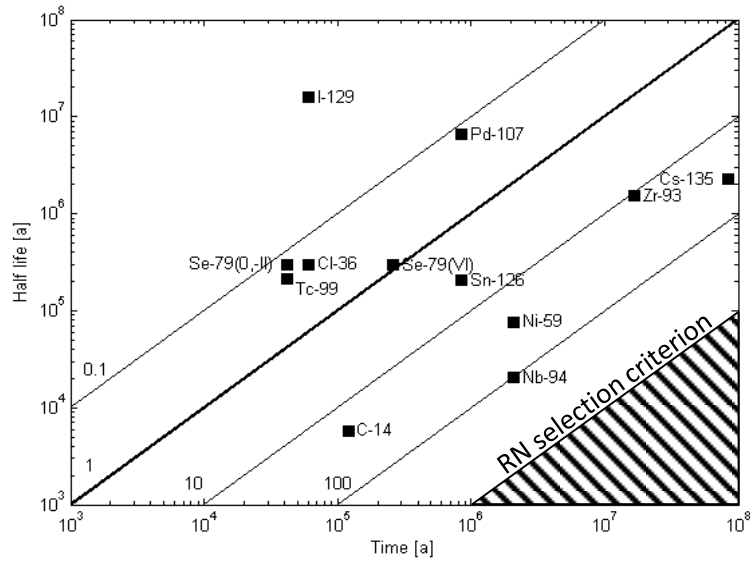


Figure 31: Radionuclide half-life versus transport time through the Boom clay layer (modified after Marivoet et al., 2010).

A2 Actinide chains

In order to significantly reduce the computational effort, actinide chains are usually represented by maximum 4 long-lived members. This is a simplification, since there are usually about eight to nine alpha decays necessary to reach the final stable isotope ($^{206,207,208}\text{Pb}$ or $^{209}\text{Bi}^{15}$). The initial inventories of some relatively short-lived radionuclides are converted into an equivalent amount of longer-lived daughter nuclides ('instant decay'). The simplified actinide decay chains considered in the simulations then become:

4N : Cm-248 → Pu-244 → U-236 → Th-232
Cm-244 and Pu-240 converted to U-236

4N+1 : Np-237 → U-233 → Th-229
Cm-245, Pu-241 and Am-241 converted to Np-237

4N+2 : U-238 → U-234 → Th-230 → Ra-226
Cm-246 and Pu-242 and converted to U-238; Pu-238, Cm-242 and Am-242 converted to U-234

4N+3 : U-235 → Pa-231
Cm-247, Am-243 and Pu-239 converted to U-235




The conversions that we consider here are for radionuclides with half-lives hundreds to few thousand years, for which inventory data are given and should be taken into account. The contribution to the radiological impact of the last radionuclides' short-lived progeny is accounted for in the biosphere compartment through the dose coefficients. In some cases, there may be a need to separately assess the impact in the biosphere compartment. This is particularly true for Pb-210, Po-210 (Ra-226 decay) and Ac-227 (Pa-231 decay).

¹⁵ In fact, ^{205}Tl is the first daughter that is considered truly stable. The half-life of ^{209}Bi is 1.9×10^{19} years.

Besides, there are some relatively longer-lived radionuclides (with a half-life >100 years), which typically are not included in the calculations. Examples of such radionuclides are those at the top of the decay chains (*e.g.*, the curium isotopes Cm-245, Cm-246 and Cm-247). Supporting calculations are needed to investigate the effect of omitting such radionuclides from the calculations.

It can be anticipated that one of the retained performance indicators will be evolution of the radiotoxicity inventory in the main compartments of the repository system. As various Pu isotopes give a considerable contribution to the radiotoxicity, it will be necessary to consider those Pu isotopes explicitly in the calculations.

In general, the treatment of the actinide chains in the host rock and in the biosphere will be further elaborated in the future.

		Date	Approval
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