Radioactive Waste Management

NDA Report no. DSSC/458/01

Geological Disposal

Criticality Safety Status Report

December 2016

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Conditions of Publication

ISBN 978-1-84029-571-9

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Abstract

The Criticality Safety status report explains contributions to safety and technical studies that support our safety cases for demonstrating criticality safety. It is one of a suite of eight research status reports that form part of the generic Disposal System Safety Case. Each research status report draws on and summarises supporting technical and scientific references in order to provide an overview of the published scientific literature for each topic. The reports have been written for an audience with a scientific or technical background and with some knowledge of the context of geological disposal. The current suite of research status reports (issue 2) updates and replaces the suite produced in 2010 (issue 1).

The objective of the Criticality Safety status report is to: define what we mean by criticality and criticality safety; summarise the contributions to safety; outline the wastes and their long-term management; show how package limits are set to avoid criticality in the short to medium term; discuss the processes that determine the likelihood of a criticality in the long-term; summarise our understanding of hypothetical post-closure criticalities and explain how one would impact on our safety case; and provide a technical summary and conclusions based on our current understanding. The key message emerging from the analysis presented in this status report is that waste packages are/will be produced to ensure that criticality is not a significant concern.

Executive Summary

The Criticality Safety status report is part of a suite of research status reports describing the science and technology underpinning geological disposal of UK higher activity radioactive wastes.

These wastes contain plutonium and uranium that are used, in pure and concentrated forms, as fuel to generate power in nuclear reactors. To do this, reactors are designed to reach and maintain a condition called criticality (a self-sustaining nuclear chain reaction). Criticality safety has been defined as protection against the consequences of an inadvertent nuclear chain reaction, preferably by prevention.

We use illustrative disposal concepts to discuss the safety provided by the geological disposal facility (GDF) in a range of potential geological environments. Our understanding of the safety provided by these concepts has been established through the large amount of research that has been conducted over several decades in the UK and by waste management organisations and research institutions overseas.

We assess criticality safety as part of safety cases that we are producing for waste transport, the construction and operational phase and following closure of the GDF. We also assess criticality safety as part of our advice to waste producers on packaging proposals.

The following high-level contributions to safety apply based on our understanding of how the waste packages and the GDF will evolve over time.

For the waste material:

- we have detailed knowledge of the inventory of radioactive wastes
- for the majority of the wastes criticality safety is not a concern; in intermediate level waste (ILW) the fissile material is normally mixed with a large excess of non-fissile material, while high level waste (HLW) contains little fissile material because it has been separated during reprocessing
- small amounts of ILW will contain separated plutonium and highly enriched uranium (HEU), but these are not present as pure materials – they are dispersed amongst other non-fissile materials
- for pure materials such as plutonium and HEU, we can design a stable wasteform that is sub-critical; depleted and natural uranium are not classed as fissile material
- most spent fuel (SF) is removed from nuclear reactors because a large proportion of the fissile content has been used up and actinides and fission products have been produced during irradiation, meaning it can no longer effectively contribute to producing power in the reactor

For the packages:

- we specify and ensures control of all waste package contents
- for the majority of SF the wasteform design is already fixed, so we will use a package design to ensure sub-critical conditions
- for packaging of HEU and plutonium at high loadings, safety will be provided by a stable, sub-critical wasteform and a long-lived container.

In all cases Radioactive Waste Management (RWM) aims to design packages that are robust to faults during transport and operations. We use well established methods with appropriate conservatisms. In the Disposability Assessment process we ensure that these packages are properly designed by assessing them against waste package specifications,

themselves derived from our generic disposal system safety case. We also ensure that the packages actually produced meet these specifications. In time, we will replace these specifications with Conditions for Acceptance.

We also assess criticality safety as part of the assessment of post-closure performance of the GDF and associated radiological risk. Depending on the type of waste, packages are designed to contain their fissile material for medium to long timescales. Over extended times, the packages will degrade as the containers corrode and a portion of the package contents may become mobilised. We consider a criticality post-closure to be unlikely; a low probability event. However, with large numbers of packages, and very long post-closure timescales requiring consideration, it is difficult to guarantee that a criticality cannot occur. Therefore we have also carried out research to understand how a criticality could begin, progress and end, including consideration of how such an event might affect the performance of the disposal system.

The likelihood of post-closure criticality is low because:

- waste containers will be emplaced in the GDF in a sub-critical configuration with multiple engineered barriers to minimise fissile material relocation
- many of the anticipated changes to the waste packages following closure are expected to reduce system reactivity
- for ILW, the fissile material is dispersed through waste packaging materials at concentrations well below critical values
- the majority of ILW is/will be encapsulated in cement, and ILW disposal concepts are based on cementitious backfill, the properties of which hinder the movement of fissile material
- for pure plutonium and uranium materials, RWM could design a wasteform that is stable and would only very slowly release fissile material
- for SF we will use a package and emplacement design capable of maintaining sub-critical conditions over long timescales and, in the majority of fuel types, the reactivity will tend to reduce with time as ^{239}Pu decays into the less reactive ^{235}U, both of which will be diluted by non-fissile ^{238}U. Furthermore, formation of critical configurations in SF containers is not possible provided the average irradiation of the fuel is above a certain amount (for example 35 GWd/tU for PWR SF).

The consequences of a post-closure criticality are low because:

- rapid transient criticality could only occur for a narrow range of hypothetical conditions, and such a criticality is not considered to be credible after about 100,000 years, due to decay of ^{239}Pu
- the consequences of a quasi-steady state (QSS) criticality are highly localised and would not affect the surrounding geosphere and therefore would not significantly impact overall risk
- direct radiation from a criticality event would be shielded by the surrounding rocks and there would be no direct risk posed to operators or members of the public
- for QSS criticality, the calculated temperature rise and power are very local and the maximum temperature would be less than a few hundred degrees Celsius, corresponding to a power output of a few kilowatts. Within a few metres the temperature rise would be of the order of degrees Celsius
- even if one were to occur, the effects of a criticality event are likely to affect only a limited part (of the order of tens of cubic metres) of the GDF

- criticality events involving very large amounts of fissile material might have a significant impact on a small fraction of the GDF, but these events are very unlikely and could only occur a long time after closure. Their effect on overall risk is small.
- the backfill/buffer and geological environment will still act to isolate the radioactive waste from the surface environment.

Based on modelling of the consequences of criticality events, and combining this with analysis of their likelihood, we consider that the risk from post-closure criticality is not a significant concern.

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List of key terminology specific to this report

***$K_{effective}$*: A useful way of quantifying how close a system is to being critical is by calculating a mathematical factor known as $K_{effective}$, the ratio of the rate of neutron production (by fission) to the rate of neutron losses (by absorption plus leakage).

Credible event: An event that is hypothetically possible and therefore has a likelihood associated with it, although (in terms of its use in this report) it is almost always considered to be of low likelihood.

Incredible event/not credible: Where the probability of an event occurring is expected (or has been demonstrated) to be vanishingly small or zero.

Package envelope: A generic “low-likelihood package envelope” (referred to as the “package envelope”) that establishes the packaging and disposal facility conditions under which post-closure criticality is considered unlikely to occur.

Deterministic calculations: Calculations in which all parameters take a single, fixed value.

Bounding calculations: Typically deterministic calculations where the single, fixed values selected are conservative or worst case.

Probabilistic calculations: Calculations in which many individual realisations are carried out – in each realisation some or all parameters take a randomly sampled value from a probability density function (PDF) representing the uncertainty in the parameter.

‘What-if’ criticality scenario: An assumed sequence of events whereby, within a localised volume of the geological disposal facility or the surrounding host rock, a critical configuration of fissile materials is reached.

Hypothetical criticality event: A specific example for a ‘what-if’ scenario whereby a critical configuration is selected for criticality consequence analysis.

Static criticality calculations: The use of criticality software to determine the neutron-multiplication factor $K_{effective}$.

Transient criticality models: The Quasi Steady State, Rapid Transient and Bounding Approach models.

Criticality consequence analysis: Use of the transient criticality models to understand the local consequences of hypothetical transient criticality events.

List of acronyms

AGR - Advanced gas-cooled reactor

ALARP - As low as reasonably practicable

AP1000 - Westinghouse Electric Company pressurised water reactor

BSO - Basic safety objective

BUC - Burn-up credit

CSA - Criticality safety assessment

CoRWM - Committee on radioactive waste management

DCTC - Disposal container transport container

DNLEU - Depleted, natural and low-enriched uranium

DSSC - Disposal system safety case

EC - European Commission

FEP - Features, events and processes

FETCH - Finite element transient criticality (the name of a computer code)

GCSA - General criticality safety assessment

gCSA - Generic criticality safety assessment

GDF - Geological disposal facility

GPA03 - 2003 Generic performance assessment

GRA - Guidance on requirements for authorisation

GSL - General screening level

GWd/tU - Gigawatt days per tonne of uranium

HEU - Highly enriched uranium

HHGW - High heat generating waste

HLW - High level waste

IAEA - International Atomic Energy Agency

ILW - Intermediate level waste

LoC - Letter of compliance

LEU - Low enriched uranium

LHGW - Low heat generating waste

LLW - Low level waste

LSL - Lower screening level

MOX - Mixed oxide

MRWS - Managing radioactive waste safely

NDA - Nuclear Decommissioning Authority

NEA - Nuclear Energy Agency within the Organisation for Economic Co-operation and Development (OECD)

NGO – Non-government organisation

NRVB - Nirex reference vault backfill

ONR - Office for Nuclear Regulation

PCCCA - Post-closure criticality consequence assessment

PCM - Plutonium contaminated material

PDF - Probability density function

PWR - Pressurised water reactor

RSC - Robust shielded containers

QSS - Quasi steady state

RT - Rapid transient

RTM - Rapid transient model

RWM - Radioactive Waste Management

SF - Spent fuel

SAP - Safety assessment principles

SWTC - Standard waste transport container

UCuRC - Understanding criticality under repository conditions

UK EPR - United Kingdom European pressurised reactor

UK RWI - United Kingdom radioactive waste inventory

USL - Upper screening level

WVP - Waste vitrification plant

1 Introduction

1.1 Background

In order to build confidence in the safety of the future geological disposal facility (GDF) for the UK[1], in the absence of potential disposal sites, RWM is developing a generic Disposal System Safety Case (DSSC), which shows how the waste inventory destined for geological disposal could be safely disposed of in a range of geological environments. Background information on geological disposal in the UK can be found in the Technical Background Document [1].

The documents comprising the generic DSSC are shown in Figure 1 and include a number of research status reports ('knowledge base'). The purpose of the research status reports is to describe the science and technology underpinning geological disposal of UK higher activity wastes by providing a structured review and summary of relevant published scientific literature and discussing its relevance in the UK context. The current suite of research status reports (issue 2) updates and replaces the suite produced in 2010 (issue 1).

Figure 1 shows how research status reports underpin different safety cases. They include:

- reports on waste package evolution [2], engineered barrier system (EBS) evolution [3], and geosphere [4], describing the understanding of the evolution of the specific barriers of the multi-barrier system
- reports on behaviour of radionuclides and non-radiological species in groundwater [5], and gas generation and migration [6], describing the release and movement of materials through the multi-barrier system, including the groundwater and any gas phase formed
- reports on criticality safety (this report) and on waste package accident performance [7], describing the behaviour of waste packages and the GDF during low probability events
- a report on the biosphere [8], describing how we think the biosphere may evolve in the future and how radionuclide uptake might be expected to take place.

Research status reports need to be read in conjunction with other documentation, including:

- the Data Report [9], which describes the values of specific parameters used in the safety assessments based on scientific information presented in the status reports
- the Science and Technology Plan [10], which describes planned future research and development activities.

1.2 Objectives and scope

The objective of the Criticality Safety status report is to explain the contributions to safety and technical studies that support our safety cases for demonstrating criticality safety of waste packages during transport, the operational phase of the facility and after disposal in the GDF.

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[1] Disposal of higher activity radioactive wastes in a GDF is current policy in England, Wales and Northern Ireland. Scottish Government policy is that the long-term management of higher activity radioactive waste should be in near-surface facilities. Facilities should be located as near to the sites where the waste is produced as possible.

The Criticality Safety Status Report shows how package fissile material limits are set to avoid criticality in the short to medium term. It discusses the processes that determine the likelihood of a criticality in the long term. It also summarises understanding of hypothetical post-closure criticalities. We assess criticality safety as part of our generic transport, operational and environmental safety cases and also in our advice to waste producers on conditioning and packaging proposals.

The scope covers all materials currently considered in the inventory for disposal, including intermediate and low level waste (ILW/LLW), high level waste (HLW), spent fuels, uranium (particularly depleted, natural and low-enriched uranium, DNLEU) and plutonium.

Figure 1 Structure of the generic Disposal System Safety Case (DSSC). The suite of research status reports represents the knowledge base

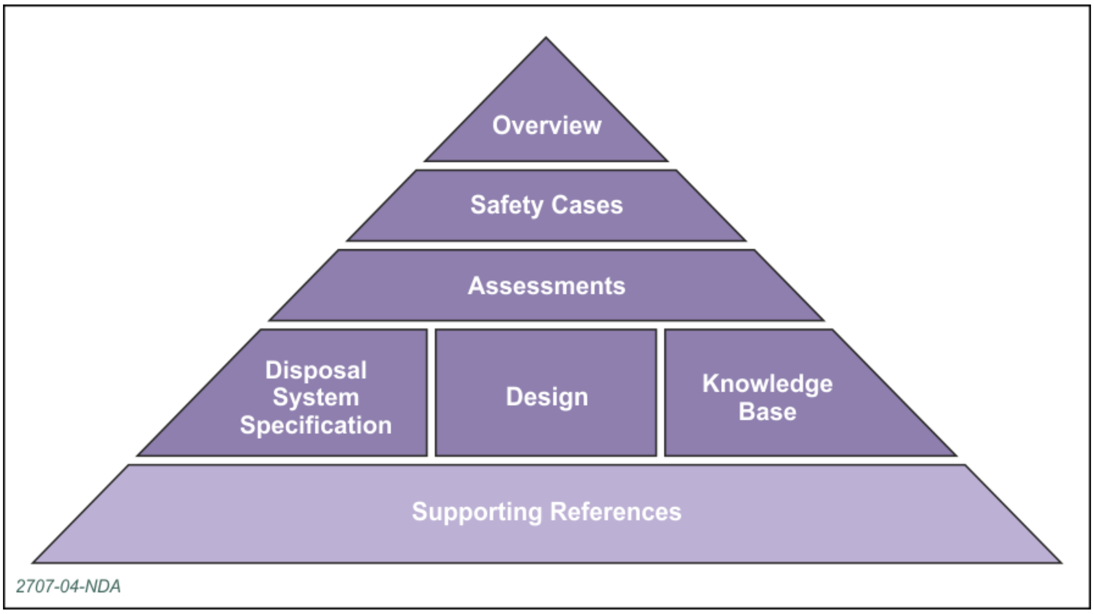
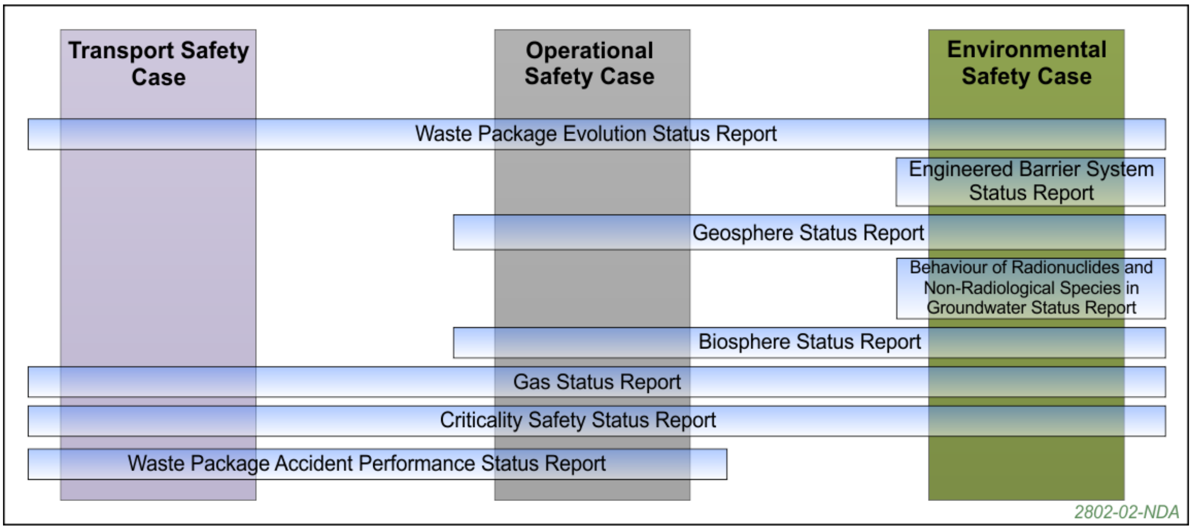


Figure 2 Safety cases and status reports in which underpinning information can be found



1.3 Audience and users

The primary external audience of the status reports is our regulators. The audience is also expected to include academics, learned societies and stakeholders such as the Committee on Radioactive Waste Management (CoRWM) and Non-Governmental Organisations (NGOs). The reports have been written for an audience with a scientific or technical background and with some knowledge of the context of geological disposal. The primary internal user of the information presented in the status reports is RWM's safety case team.

1.4 Relationship with other status reports

There are important interfaces between this and other research status reports. Information providing underpinning to the Criticality Safety status report includes:

- the expected evolution of various wasteform and waste container materials, which is discussed in the Waste Package Evolution status report [2]. This is a key input to our post-closure criticality considerations, as it influences the timeframe on which fissile material could be released from waste packages and mobilised within the near field of the GDF.
- The Engineered Barrier System status report [3], as post-closure criticality considerations depend strongly on our understanding of the expected evolution of conditions in the near field of the GDF and the migration of fissile radionuclides over long time periods.

1.5 Changes from the previous issue

This document updates and replaces the 2010 Criticality Safety status report [11], published as part of the 2010 generic DSSC suite. This issue includes the following developments:

- an explanation of the revised position for setting post-closure derived package fissile limits/levels
- recent work on package fissile limits for robust shielded containers (RSC)
- recent work on the disposal container transport container (DCTC)
- a new section detailing scenarios for post-closure safety assessment
- a rewritten and expanded section presenting recent results on the likelihood of criticality
- a rewritten and expanded section presenting recent results on the consequences of hypothetical criticality
- an update of the generic post-closure criticality consequences assessment (PCCCA).

1.6 Knowledge base reference period

The knowledge base described in this document contains scientific information available to RWM up to March 2016. Where, within RWM's research programme, progress relative to important topics was made after such date, efforts have been made to reflect such progress up to the publication date of this document.

1.7 Document structure

The remainder of this report is structured according to the following format:

- Section 2 introduces the nature of the criticality hazard, defines criticality safety, and summarises the contributions to safety during transport, pre-closure operations and the post-closure phase of GDF
- Section 3 shows how limits are set to specify, and enable control of, waste package contents
- Section 4 discusses the processes that are relevant in determining scenarios that could give rise to a post-closure criticality, noting the importance of the barriers provided by the waste package, the backfill, and the surrounding geology; we outline the scenarios for post-closure criticality that we have used in assessments of the likelihood and consequences of criticality
- Section 5 provides a summary of our work to estimate the likelihood of criticality for various scenarios, describes the methodology and models used for the analysis, including their limitations, and presents arguments about the likelihood of criticality for different types of waste
- Section 6 summarises our understanding of the consequences of post-closure criticality, outlines the models that have been developed to predict the consequences of a postulated criticality and indicates the role of these models in the overall assessment of post-closure risk
- Section 7 links the research on likelihood and consequences of criticality to the implications for post-closure safety
- Section 8 provides a technical summary and conclusions based on our current understanding.

We have used coloured boxes at the beginning of each section to provide a short summary of the key messages and help the reader in following the ‘golden thread’.

2 Criticality Safety in Waste Management and Disposal

In this section we:

- define what we mean by criticality and criticality safety
- list the means by which criticality may be prevented
- briefly outline the consequences to the GDF if a criticality should occur post-closure
- identify the relevant contributions to safety that underpin the arguments made in the criticality safety cases
- discuss our broad approach used to demonstrate criticality safety for waste management operations.

2.1 Nature of criticality hazards

If enough fissile material were to be brought together in the GDF by some mechanism an uncontrolled nuclear chain reaction (criticality) might occur. Two broad types of criticality event are hypothetically possible, each characterised by significantly different durations and consequences.

When some heavy radionuclides absorb a neutron they may split into two smaller radionuclides, releasing energy and several neutrons in the process. This is called nuclear fission. In a system containing fissile[2] material, the neutrons released may go on to produce more neutrons by further fission or be lost through absorption in non-fissile radionuclides, or may leave the fissile part of the system to be absorbed in surrounding materials (a process referred to as leakage). In certain very specific configurations a self-sustaining neutron chain reaction of fission can be established. When controlled, this is the process by which heat/energy is produced in a nuclear power plant.

If enough fissile material (both in quantity and concentration) were to be brought together outside the carefully engineered environment of a nuclear reactor core an uncontrolled chain reaction might occur, releasing dangerous amounts of radiation to anyone in close proximity, and in certain circumstances, producing significant amounts of energy. This type of uncontrolled event is known as a criticality accident. Criticality safety can be defined [12] as protection against the consequences of an inadvertent nuclear chain reaction, preferably by prevention of the chain reaction.

At the point where the chain reaction becomes self-sustaining the system is said to be critical and there is a balance between the number of neutrons being produced by fission and the numbers being lost by absorption and leakage. In this condition the fission rate is steady. If the number of neutrons produced by fission exceeds the numbers being lost, the neutron population and fission rate will increase and the system is said to be super-critical. In a sub-critical system neutron losses exceed neutron production so that a chain reaction cannot be sustained.

A useful way of quantifying how close a system is to being critical is by calculating a mathematical factor known as $K_{effective}$, the ratio of the rate of neutron production (by fission) to the rate of neutron losses (by absorption and leakage). At the point of criticality $K_{effective}$ is

2 This report focuses on wastes that contain substantial amounts of ^{239}Pu and ^{235}U, which are the key fissile radionuclides present (fissionable radionuclides that can undergo fission with low energy neutrons). Radionuclides that fission predominantly as a result of interaction with fast neutrons are not considered to present a criticality concern in the GDF because disposal systems are expected to be moderating (and potentially over-moderating) in the presence of waste materials and water.

equal to unity (1.0). For super-critical systems $K_{effective}$ is greater than 1.0, and it is less than 1.0 for sub-critical systems. The ‘reactivity’ of a fissile system is a measure of the departure of $K_{effective}$ from unity.

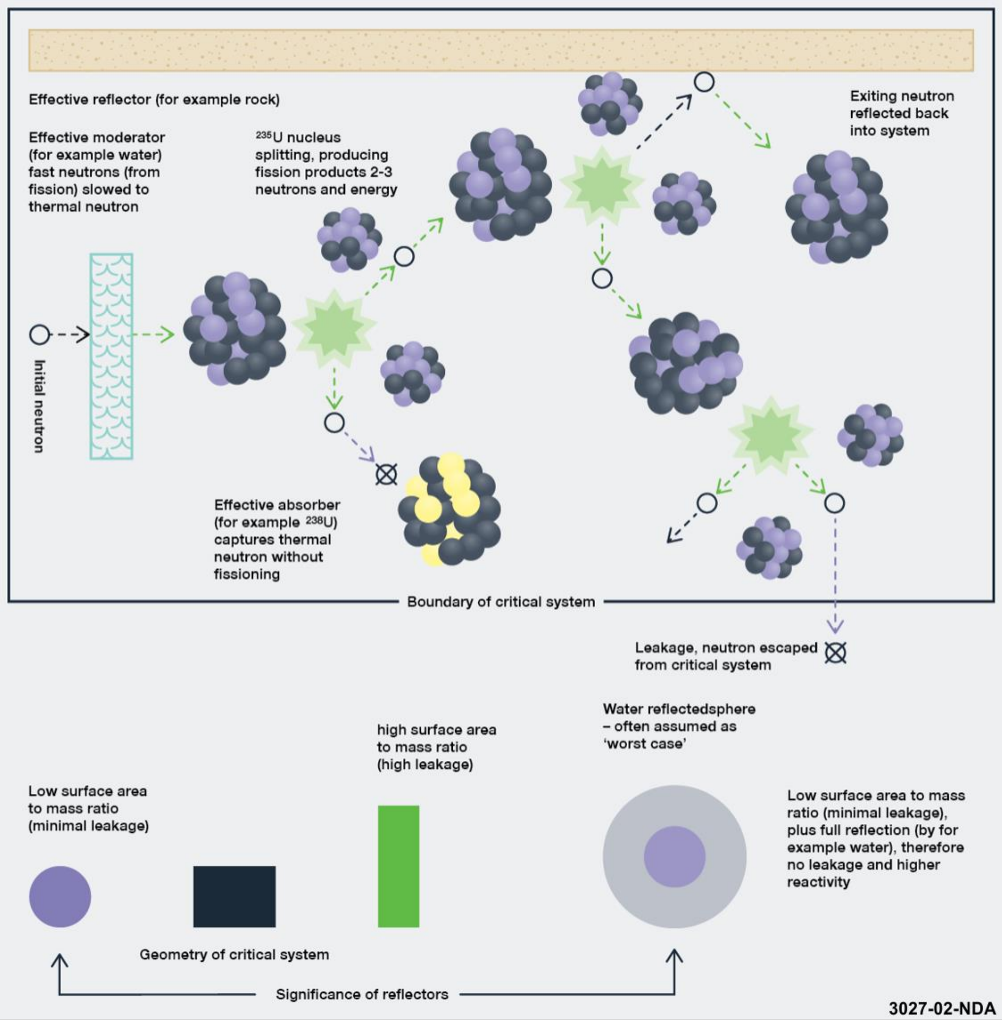
The balance between neutron production and neutron absorption/loss, which is the key to ensuring criticality safety, is influenced by many factors. The factors generally found to be most useful in imposing criticality safety control include:

- mass, density, volume, geometry
- concentration, enrichment
- moderation, absorption, reflection and
- interaction[3].

3 Neutron interaction concerns multiple fissile units (or waste packages), each of which is subcritical in isolation. However, the combined system may be critical due to the interaction between the units, that is, the transfer of neutrons between units. In cases where interaction effects may be important, safety measures are put in place to ensure criticality safety.

Box 1 Introduction to critical systems

The interplay between nuclear fission and system moderation, absorption, reflection, geometry and leakage is illustrated below:



A neutron **moderator** is a medium (such as water, graphite or polythene) that reduces the speed of fast neutrons, turning them into thermal neutrons. This process dramatically increases the probability of neutron capture leading to fission.

A neutron **absorber** is a medium (such as boron or ^{238}U) with a large neutron absorption cross-section[4] that allows it to capture neutrons. The presence of efficient neutron absorbers therefore decreases the $K_{effective}$ of a system.

A neutron **reflector** is a medium (such as rock) that possesses a high scattering cross-section and a low absorption cross-section. Such media are capable of changing neutron direction. Reflectors on systems reduce leakage and therefore increase $K_{effective}$.

Leakage is the escape of neutrons from a fissile system. Leakage is reduced and neutron **interaction** increased if an efficient reflector is present.

In criticality safety assessment, **optimally moderated and fully water-reflected spheres** are often conservatively assumed to occur, as they tend to bound any likely accumulation of fissile material (or are broadly the highest reactivity system), since a sphere is generally the most reactive (lowest surface area to volume) **geometry.**

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4 The concept of a neutron cross-section is used to express the likelihood of interaction between an incident neutron and a target nucleus.

By limiting one or more of these factors, operations involving fissile material can be maintained in a sub-critical condition. Failure to maintain sub-critical conditions, mainly as a result of human error, has been the cause of about 60 criticality accidents worldwide, resulting in 21 known fatalities [13]. Of these 60 criticality accidents 22 occurred in fissile material processing facilities, and thus occurred in facilities not designed to manage critical conditions, whilst 38 occurred during criticality experiments or operations with research reactors. Importantly, with regards to waste management and geological disposal of solid wastes, 21 of the 22 known process accidents occurred when fissile material was contained within solutions or slurries, meaning that the geometrical arrangement was not necessarily fixed, so geometry could not necessarily be relied upon to ensure sub-critical conditions. Nearly all of these accidents occurred during the early years of the nuclear industry, particularly during the 'Cold War' years. In all cases significant radiological effects were limited to operators working within a few metres of the event.

During transport to, and the operational phase of, the GDF, workers (and members of the public in the case of transport) need to be protected against exposure to radiation from a criticality accident. This is generally achieved through the production of waste packages that will remain sub-critical. Following closure of the GDF, deterioration of the physical containment provided by the waste packages, movement of fissile material out of the waste packages and subsequent accumulation into new configurations could in principle lead to a criticality. At this stage there will be no operators present and any radiation produced during the criticality would be safely shielded by the surrounding rock. The issue therefore then becomes the potential effects of a criticality event on the post-closure performance of the repository system.

In the unlikely event that enough fissile material is brought together during the post-closure phase of the GDF by some mechanism, broadly two types of criticality event are hypothetically possible, each possessing significantly different timescales and consequences.

Briefly, in the first type of criticality event, referred to as a quasi-steady state (QSS) criticality, an increase in temperature causes a decrease in the reactivity of the fissile material (a negative temperature feedback). Assuming that further fissile material is still accumulating (for example, from in-flowing groundwater) this allows a steady state to be reached, often with only a modest rise in temperature, in which a 'just-critical' configuration is maintained. This just-critical configuration could last for many millennia, but would only yield physical consequences (temperature rise and power) that are typically limited to a few kilowatts of power, and a maximum temperature rise of a few hundred degrees Celsius. Therefore consequences from a QSS criticality are not expected to significantly impact the surrounding geosphere (rock properties). Furthermore, it would only impact a highly localised region.

In the second type of criticality, known as rapid transient (RT) criticality, an initial increase in temperature causes an increase in the reactivity (a positive temperature feedback). In these circumstances it is not possible to maintain a 'just-critical' configuration, so the neutron flux and power rise, leading to a rapidly escalating temperature. At some point the pressure will become sufficient to drive expansion of the critical region, leading to possible damage to the surroundings (such as possible void formation in the near field and cracking of the surrounding geosphere). This expansion may be sufficient to terminate the criticality. The timescale for a rapid transient event, from start to finish, is typically less than one second.

Importantly, the majority of hypothetical criticality events from fissile accumulation would only evolve as a QSS criticality. Post-closure RT criticality is only thought to be credible over a narrow range of ^{239}Pu concentrations (and not from predominantly uranic systems) [14]. Therefore, the passage of time lowers the possibility of rapid transient criticality occurring (as ^{239}Pu decays to ^{235}U), and after 100,000 years have passed (or about four half-lives of ^{239}Pu) RT criticality is no longer thought to be credible.

A more detailed discussion of these two types of criticality event is given in Section 6.

It is therefore hypothetically conceivable that a post-closure criticality could adversely affect the performance of a GDF because the heat and energy released might be sufficient to affect engineered barriers designed to contain the radionuclides in the waste. This is considered as part of the post-closure safety assessment [15] and is discussed further in Section 7.

2.2 What do we mean by criticality safety?

Criticality safety can be defined as protection against the consequences of an inadvertent nuclear chain reaction, preferably by prevention of the chain reaction.

We describe something as being 'safe' if we can demonstrate that there is little risk associated with it, or that we can manage the situation to keep the risk to an acceptable level. Criticality safety has been defined as protection against the consequences of an inadvertent nuclear chain reaction, preferably by prevention of the chain reaction [12]. To do this we impose limits on the contents of waste packages containing fissile material such that they will remain sub-critical in all normal and credible accident conditions.

The design of the wasteform and packages, and the conditions during transport and emplacement, provide a series of layers of defence, ideally to prevent a criticality occurring at all, or by limiting its consequences if such an event cannot be ruled out entirely. This concept of 'defence-in-depth' is central to our approach to criticality safety.

Evidence from criticality accidents shows us that most have been caused, to a greater or lesser extent, by failure of safety measures relying on operator actions [13]. Where practicable this type of protection should be avoided, and the aim is to provide layers of defence based on passive features of the design (for example, the dimensions and shape of containers, or some inherent property of the fissile material like low fissile concentration) to prevent a critical system being formed.

If it is not practicable to establish this type of deterministic demonstration of safety, criticality safety must be demonstrated through a probabilistic approach. Probabilistic assessments are based on estimating the risk associated with certain processes, given the uncertainties. Here risk is defined as the product of the frequency of an event multiplied by its consequences.

The requirements for criticality safety assessment of various phases of the disposal route are specified by the relevant regulatory bodies. Safe transport of fissile materials to the GDF will be addressed by our transport safety case [16] and regulated by the Office for Nuclear Regulation (ONR) following international regulations established by the International Atomic Energy Agency (IAEA) [17]. During transport there is potentially a hazard to members of the public and there is strong emphasis on deterministically demonstrating that a criticality cannot occur in normal, or any credible, accident conditions.

The safety of operations on licensed nuclear sites (including at a future GDF) is also regulated by the ONR. A fundamental requirement of the ONR is that the risks associated with proposed operations must have been demonstrated to be 'As Low As Reasonably Practicable' (ALARP) [18]. In the context of criticality safety this may be by showing that there is sufficient defence in depth, or through a probabilistic argument showing that risks comply with numerical targets. Our operational safety case [19] must also show that any further risk reduction could only be made at a cost considered to be grossly disproportionate to the benefit achieved.

Once the GDF has been closed regulatory responsibility falls under the relevant environment agency. At this stage the risk of direct radiation exposure to operators or the public is removed due to the location of the material deep underground in an engineered facility. However, criticality might conceivably affect the ability of the GDF to contain the radionuclide inventory and the environmental safety case must therefore demonstrate that:

> '*The possibility of a local accumulation of fissile material such as to produce a neutron chain reaction is not a significant concern.'*

Furthermore, RWM as the implementer is also required to investigate as a 'what-if' scenario:

> *'The* impact *of a postulated criticality event on the performance of the disposal system.'*

These requirements are expressed in the environment agencies'[5] 'Guidance on Requirements for Authorisation' (GRA) [20].

2.3 Contributions to safety

We need to demonstrate criticality safety both prior to closure of the GDF (during transport and operations) and following GDF closure.

This section identifies the relevant contributions to safety that underpin the arguments made in the criticality safety cases.

Criticality is a key FEP (features, events and processes) in the NEA FEP list [21]. The work presented in this report summarises our full understanding of this important FEP. A detailed and structured approach is used in our studies of the likelihood of criticality post-closure (see Section 5). Also, it is implicit in the approach to criticality safety in earlier phases of waste management. The outputs of these approaches are presented here as the main contributions to safety during pre-closure operations, which are discussed in subsection 2.3.1, and those following closure, which are discussed in subsection 2.3.2.

2.3.1 Pre-closure operations

Prior to GDF closure, in most cases, criticality control is based on limiting the fissile content of packages (for example for ILW) and/or controlling the geometry of the fissile distribution (for example for SF). The robust nature of the packages ensures that rearrangement of the fissile component into an unsafe configuration cannot occur during transport or operations.

Operations involving processing, storage and transport of fissile material in the form of nuclear fuel have been subject to criticality assessment over many years using well established methodologies. The general principles of those methodologies are also applicable to the assessment of similar operations on fissile waste. Responsibility for the production of safety cases for conditioning, packaging and interim surface storage of these materials lies with the site operators of those facilities.

We assess criticality safety as part of the safety cases for transport to and operation of the GDF. We also assess criticality safety, as part of our advice to site operators on conditioning and packaging proposals through the Letter of Compliance Disposability

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5 The Environment Agency, the Scottish Environment Protection Agency (SEPA) and the Northern Ireland Environment Agency (NIEA) are responsible for regulating the disposal of radioactive waste in England and Wales, in Scotland, and in Northern Ireland respectively. The GRA referred to was issued by the Environment Agency and the NIEA. For simplicity this report uses the term environment agencies', but in reality it only refers to these two organisations.

Assessment process, to ensure that every waste package will comply with the requirements of the Disposal System Specification [22] and the Waste Package Specifications [23, 24]. The contributions to safety listed in Box 2 apply in some or all of these safety cases.

Box 2 Pre-closure contributions to safety

For the waste material:

- RWM has a detailed knowledge of the inventory of radioactive wastes and materials.
- for the majority of the wastes criticality safety is not a concern. In ILW the fissile material is nearly always mixed with a large excess of non-fissile material. HLW contains little fissile material because this has been separated during the reprocessing of SF.
- small amounts of ILW will contain separated plutonium and HEU, but these are not present as pure materials – they are dispersed amongst other non-fissile waste materials.
- for pure materials such as plutonium and HEU, RWM can design a stable wasteform that is sub-critical.
- most spent fuel (SF) is removed from nuclear reactors because a large proportion of the fissile content has been used up and actinides and fission products have been produced during irradiation, meaning it can no longer effectively contribute to producing power in the reactor.

For the packages:

- RWM specifies and ensures control of all waste package contents.
- for the majority of SF, the wasteform design is already fixed by the nature of the waste, that is, it comprises a metallic or ceramic fissile material surrounded by cladding, so we will use a package design to ensure safe sub-critical conditions (for example, this might include using materials that absorb neutrons to prevent criticality).
- for packaging of HEU and plutonium at high loadings, (for example, in the current packaging assumption of a ceramic wasteform emplaced in the HLW disposal area), contributions to safety will be provided by the stable, sub-critical wasteform and a long-lived container.
- in all cases, we aim to design packages that are robust to faults during transport and operations.

In most cases, criticality control is based on limiting the fissile content of packages (for example for ILW) and/or applying geometric control of the fissile distribution (for example for SF). Once the waste containers are loaded, the robust nature of the packages ensures that rearrangement of the fissile component into an unsafe configuration cannot occur during transport or emplacement. The process applied to derive safe package fissile material limits is discussed in Section 3.

2.3.2 Post-closure

After GDF closure, package fissile material limits will help to prevent a criticality for a considerable time. Once packages have degraded, we aim to demonstrate that the likelihood and consequences of post-closure criticality (following a reconfiguration and/or accumulation of fissile material) are both low.

Packaging, and package limits, will help prevent a criticality for such time as the waste packaging affords a high level of containment. However, once the GDF is sealed these engineered measures will start to degrade as the containers corrode; a portion of the package contents may eventually become mobilised by groundwater.

In contrast to preceding phases of the disposal route, criticality safety for the entire duration of the post-closure phase of the GDF (perhaps a million years) cannot readily be demonstrated in a deterministic assessment of the protection offered by engineered measures and fixed package limits. In the post-closure assessment there is necessarily more reliance on probabilistic arguments in order to demonstrate that the likelihood and consequences of post-closure criticality are both low.

The contributions to safety listed in Box 3 apply in the post-closure criticality safety case.

Box 3 Post-closure contributions to safety

The likelihood of post-closure criticality is low because:

- waste containers will be emplaced in the GDF in a sub-critical configuration, with multiple engineered barriers in place to retard the effects of processes that might lead to significant relocation of fissile material.
- many of the anticipated changes in the evolution of waste packages in this environment following closure are expected to reduce system reactivity.
- for ILW, the fissile material is well spread out; the total fissile content of 13.5 tonnes being dispersed through ~470,000 m^3 of waste packaging materials, at concentrations well below critical values.
- the majority of ILW is/will be encapsulated in cement, and ILW disposal concepts are based on cementitious backfill, the chemical and physical properties of which hinder movement of fissile material.
- for pure plutonium and uranium materials, which are not yet categorised as wastes, RWM could design a wasteform that is stable for long times and would only very slowly release fissile material, as in the current packaging assumption.
- for SF we will use package and emplacement designs capable of maintaining sub-critical conditions over very long timescales and, in the majority of fuel types, the reactivity will broadly reduce with time as ^{239}Pu decays into less reactive ^{235}U, both of which will be diluted by non-fissile ^{238}U. Furthermore, formation of critical configurations in SF containers is not possible provided the average irradiation of the fuel is above a certain amount (for example 35 GWd/tU for PWR SF).

The consequences of post-closure criticality are low because:

- rapid transient criticality could only occur for a narrow range of hypothetical conditions, and such a criticality is not considered to be credible after about 100,000 years post-closure, due to decay of ^{239}Pu to ^{235}U.
- for a QSS criticality, the physical consequences are highly localised and would not be expected to affect the surrounding geosphere, and therefore would not significantly impact on overall risk.
- direct radiation from a criticality event would be shielded by the surrounding rocks and materials. Unlike during the transport or operational phases of the GDF there will be no direct risk posed to operators or members of the public.
- for QSS criticality, the calculated temperature rise and power are less than 300 °C locally and a few kilowatts, irrespective of whether the underlying scenario is accumulation, stack slumping or in-package flooding.
- even if such were to occur, criticality events are likely to affect only a limited part (of the order of tens of cubic metres) of the GDF.
- criticality events involving very large amounts of fissile material might have a significant impact on a small fraction of the GDF and the engineered barrier system, but these events are very unlikely and could only occur a long time (hundreds of thousands of years) after closure, when the radioactive inventory will have decayed to much lower levels. Therefore their effect on the overall risk will be small.
- the backfill/buffer and geological environment will still act to isolate the radioactive waste from the surface environment.

We have carried out a detailed research programme to provide technical underpinning for these arguments. In particular we aim to demonstrate that both the likelihood and consequences of a post-closure criticality event are low and therefore are not of significant concern. The evidence provided by these studies is summarised in Sections 5, 6 and 7.

2.4 Approach to demonstrating criticality safety

Our overall understanding of the processes affecting criticality safety involves complementary types of investigation, comprising analysis of existing knowledge, modelling using both widely used and specially created software, and analysis of a natural analogue.

Almost all of our studies are modelling, supported by existing knowledge. Criticality experiments have been conducted and documented, mostly in facilities that are no longer operational. Analysis and re-analysis continues to this day, for example in the International Criticality Safety Benchmark Evaluation Project [25]. This supports the validation of neutron transport codes that are used in our criticality safety assessments, for example to demonstrate the criticality safety of SF in transport containers [26] and of waste in robust shielded containers [27]. Unplanned criticalities have been analysed internationally, mainly to learn lessons to avoid further events [13], but also to confirm limits on key parameters and to support predictions of consequences.

Super-critical experiments are represented in historical underground testing, the consequences of which were documented [28,29] and have been analysed as part of our research programme [30].

Modelling is used in a number of ways to build understanding of criticality safety. For example, modelling of SF assemblies, in specified geometries during normal and accident conditions of transport, formed a major part of the DCTC analysis [26]. The models used the internationally recognised and validated neutron transport code MONK [31].

The evolution of waste packages and migration of fissile material post-closure has been modelled using GoldSim [32,33] to assess the likelihood of criticality post-closure [34]. It is not always possible to validate such post-closure computer models, due to, for example the long post-closure timescales of interest meaning that you cannot make use of real time experiments. You can, however, use natural analogues and other studies to build confidence in the model. The Oklo natural reactors [35,36] (see subsection 4.9) present just such a natural analogue, the analysis of which [37] has been used to build confidence in an approach that models the post-closure consequences of hypothetical accumulations of fissile material [38].

3 Ensuring Criticality Safety in Radioactive Waste Management

In this section we:

- review the fissile content of the waste inventory
- discuss how we ensure waste packages are compliant with fissile controls using the Disposability Assessment process and how this supports our DSSC
- discuss our approach to setting package fissile material limits and summarise the criticality scenarios considered for the transport and GDF operational[6] and post-closure phases
- outline the hierarchy of package fissile material limits for LLW, ILW and DNLEU, and discuss the developing methodology for post-closure criticality assessment
- consider the approach for ensuring criticality safety for HLW, SF, and separated HEU and plutonium, and discuss areas of ongoing and future research.

It is essential that appropriate criticality controls are established for all radioactive waste management operations from conditioning, packaging and interim storage through to transport, emplacement and eventual disposal in the GDF. Adherence to this principle helps to ensure that unnecessary repackaging is avoided. RWM is, however, only responsible for the three distinct phases of the GDF's lifecycle: transport to the facility, operations at the facility and the eventual post-closure phase. We show here how knowledge of the waste inventory, control over the wasteform and waste packaging, and an understanding of the range of normal and accident conditions that might credibly be encountered, all contribute to safety and are combined to provide the basis for setting appropriate criticality controls.

In subsection 3.1 we review the nature of the waste materials that may require geological disposal from a criticality safety point of view. Subsection 3.2 discusses how we ensure that waste packages are compliant with criticality controls, such as fissile material limits, and how this supports our DSSC. Subsection 3.3 discusses RWM's approach to setting package fissile material limits and summarises the types of criticality scenarios assessed for each of the three GDF phases. Subsection 3.4 outlines the hierarchy of package fissile material limits for LLW, ILW and DNLEU, and expands on the developing methodology for post-closure criticality safety assessment. Subsections 3.5 and 3.6 consider the approach for ensuring criticality safety for HLW and SF, and separated HEU and plutonium, respectively.

3.1 Nature of the materials

^{235}U and ^{239}Pu are the main fissile radionuclides present in radioactive waste. They are present in significant quantities in ILW and LLW, spent fuel, plutonium and uranium wastes/materials.

This subsection reviews the waste inventory from a criticality safety point of view. Information on the mass and effective average enrichment of the principle fissile radionuclides (^{235}U and ^{239}Pu) present in each of the inventory waste groups is presented.

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6 The GDF operational period is typically assumed to last 50-150 years and this range depends on which part of the facility is being considering.

The waste inventory for disposal in the GDF is comprised of hundreds of waste streams, which include a range of radionuclides and materials, and will be packaged in a number of forms and waste containers. A criticality safety assessment must consider the mass and concentration of fissile material in each waste package, as well as the presence of any neutron moderating, absorbing or reflecting materials.

The radionuclides ^{235}U and ^{239}Pu are the main fissile radionuclides present in radioactive waste. Other fissile radionuclides are present in radioactive waste but in LLW/ILW, for example, only ^{233}U and ^{242m}Am will be present at 2150 (an indicative closure time for the GDF) in quantities greater than the relevant minimum critical mass. Inventory data indicates that these nuclides will be dispersed over many waste packages in quantities of less than a few grams per package and such masses are unlikely to present a criticality concern[7]. To give a similar example from the SF/HLW inventory, of the remaining fissile nuclides only ^{241}Pu, ^{242m}Am, and ^{245}Cm are present in total quantities that are greater than the relevant minimum critical mass. It is expected that these nuclides would be dispersed in small quantities amongst wastes in many packages, and that the likelihood that they would contribute significantly to any accumulation of fissile material after disposal is negligible.

The 2013 Derived Inventory of wastes and materials is summarised in [39] in terms of total volume and radioactivity. Table 1 presents the 2013 Derived Inventory in terms of the masses of uranium and plutonium. The average fissile enrichment across the entire waste category ((^{239}Pu+^{235}U)/(Total Pu+U)) is also calculated. However, note that the fissile mass, concentration and enrichment vary considerably between waste streams in each waste group, and there may also be considerable variation between packages in a waste stream, particularly for ILW. This variation in fissile content between waste packages in a waste stream must be accounted for in individual criticality safety assessments.

7 Note that LLW/ILW will also include potentially significant amounts of the fissile isotope ^{241}Pu at the time of disposal, but ^{241}Pu has a short half-life (14.4 years) and will have decayed to insignificant quantities by the time of GDF closure. It should also be noted that ^{241}Pu decays to ^{241}Am, then ^{237}Np and eventually fissile ^{233}U. An outstanding ^{233}U research need is discussed further within subsection 6.1.

Table 1 2013 Derived Inventory in terms of masses of uranium and plutonium at 2200 [39]. LLW intended for disposal in the GDF is included alongside legacy ILW

Waste Category	Waste Group	Packaged volume (m^3)	^{239}Pu (tonnes)	Pu-total (tonnes)	^{235}U (tonnes)	U-total (tonnes)	Average fissile enrichment (wt%)
ILW / LLW	RSC‡	7,280	0.00132	0.00215	0.0065	3.17	0.2
	SILW / SLLW†	93,000	0.000277	0.000336	0.00239	0.244	1.1
	UILW / ULLW†	327,000	6.08	7.78	7.39	1,500	0.9
	New build ILW-S†	18,900	0.0000242	0.0000397	0.0000199	0.00319	1.4
	New build ILW-U†	22,100	0.0000249	0.0000558	0.000134	0.0146	1.1
	Total ILW (inc. LLW)	468,000	6.08	7.78	7.40	1,500	0.9
HLW	HLW	9,290	0.106	0.193	0.0123	2.11	5.1
Spent Fuel	Legacy SF	14,800	21.0	37.7	40.7	6,040	1.0
	New build SF	39,400	90.6	162	78.0	13,300	1.3
	MOX	11,900	39.5	73.3	1.84	1,290	3.0
	Total SF	66,100	151	273	121	20,600	1.3
Other Nuclear Materials	DNLEU	109,000	0.00000806	0.0000121	523	184,000	0.3
	HEU	2,470	0	0	21.8	22.9	95
	Plutonium	620	4.56	5.52	0.0311	0.0588	82

‡Robust shielded containers for ILW.
†Shielded and unshielded ILW/LLW waste groups.

ILW/LLW

The total inventory of ILW (including LLW destined for the GDF) contains ~6.1 tonnes ^{239}Pu and ~7.4 tonnes ^{235}U from current stocks and predicted future arisings. Detailed examination of all the ILW/LLW streams in the 2013 Derived Inventory indicates that ~50% of the ^{239}Pu and ~85% of the ^{235}U is present as fuel residues and as such remains intimately mixed with the ~1500 tonnes of ^{238}U, which is a diluent and neutron absorber in moderated systems.

Approximately 2.9 tonnes of ^{239}Pu is present in separated form as Plutonium Contaminated Material (PCM), distributed across thirteen different waste streams that comprise mainly paper, plastics and metals with surface contamination.

Less than one tonne of ^{235}U is present in the total ILW/LLW inventory at enrichments higher than ~3 wt%, that is, at enrichments higher than those associated with irradiated light water reactor fuel residues.

HLW

The aim of reprocessing SF is to separate and recover plutonium and uranium from the fission and activation products. The wastes from this process form ILW (mainly as fuel cladding and PCM) and HLW (which contains fission and activation products). Therefore, HLW contains very little plutonium and uranium by mass, as is evident from Table 1. Assuming this waste is vitrified into ~2400 containers [39], the average fissile content is ~45 g ^{239}Pu and ~5 g ^{235}U (of total enrichment ~5 wt%), which does not represent a criticality safety concern.

Spent fuel

Three different broad categories of spent fuel are included in the 2013 Derived Inventory:

- legacy SF consists of those arisings from the Advanced Gas-cooled Reactor (AGR) fleet that will not be reprocessed, arisings from the Sizewell B Pressurised Water Reactor (PWR), metallic spent fuels (primarily some Magnox spent fuel assumed to be destined for the GDF) and exotics.
- new build SF is assumed to arise from a new nuclear power station programme using PWRs such as Westinghouse Electric Company AP1000s and United Kingdom European Pressurised Reactors (UK EPRs)[8]. Such fuel is assumed to be manufactured from fresh uranium in the form of enriched UO_2.
- ongoing work is looking at a range of options[9] for re-using the majority of the UK stockpile of separated plutonium in civil reactor mixed oxide (MOX) fuel [40]. The most viable and cost-effective option is yet to be established but, for the purposes of the 2013 Derived Inventory, RWM has assumed that the stockpile will be used to create Light Water Reactor (LWR) MOX fuel that, when spent, will require disposal in the GDF.

The total masses of fissile material in SF in the 2013 Derived Inventory are ~20 times greater than in ILW and are contained in a much smaller volume. The average residual fissile enrichment is 1.3 wt%. Little of the legacy commercial fuel in the Derived Inventory is expected to have high residual enrichments, because fuel is designed so that it is discharged from the reactor when it can no longer efficiently sustain criticality (that is, it is ‘burnt-up’). As such, these spent fuels do not present a significant criticality safety concern. However, MOX fuel and some non-commercial fuels (such as fuels from research reactor programmes) included in the Derived Inventory will possess higher average residual fissile enrichments. Our estimates of the inventories of these materials is based on certain assumptions about legacy and new build reactor operations, as presented in [39] and will require confirmation prior to disposal.

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8 The 2013 Derived Inventory assumes that a new build programme exists that generates an electrical output of 16 GW(e). Such an output is assumed to be produced from six UK EPRs and six AP1000 reactors.

9 Three ‘credible options’ for re-use of the UK stockpile of separated plutonium are currently being considered: reuse as MOX fuel in LWRs (‘LWR MOX fuel’), reuse in CANDU EC6 reactors (‘CANMOX fuel’) and reuse (as metallic fuel) in PRISM fast reactors (‘PRISM fuel’). Conversion of the plutonium into a ceramic wasteform using Hot Isostatic Pressing (‘Pu HIP’) is also being considered as an alternative to re-use (see Waste Package Evolution Status Report [2]). The 2013 Derived Inventory assumes the LWR MOX fuel option for planning purposes.

Plutonium, HEU and DNLEU

Table 1 also includes around 5.5 tonnes of separated plutonium residues that are unsuitable for future MOX fuel production. Such material is currently stored as solid PuO_2 powder and it is assumed that this is the form of the material that will be disposed of after conversion to a suitable wasteform [39].

The information on uranium in Table 1 is dominated by large volumes of depleted uranium with lesser amounts of natural, low enriched and highly enriched uranium[10]. It is assumed that HEU for disposal will be in the form of uranium dioxide (UO_2) and that DNLEU will be in the form of triuranium octaoxide (U_3O_8)[11] [39].

3.2 Disposability Assessment process

The waste package content of fissile material, neutron moderator and reflector material are controlled through the Disposability Assessment process to ensure that: criticality during transport is prevented, the risk of criticality during operations is tolerable and ALARP, and the likelihood and consequences of post-closure criticality are low.

In order to comply with the regulatory requirements for criticality safety discussed in subsection 2.2, RWM requires that the presence of fissile material, neutron moderators and reflectors in the waste package is controlled to ensure that [41]:

- criticality during transport is prevented
- the risk of criticality during the GDF operational period is tolerable and ALARP
- in the GDF post-closure period both the likelihood and consequences of criticality are low.

We ensure that criticality safety requirements are complied with through detailed knowledge of the waste materials and any conditioning carried out prior to packaging, and through careful control of the packaging process. Waste package compliance with the criticality safety requirements is assessed through our Disposability Assessment process. We established this Disposability Assessment process [42] to support those responsible for the packaging of higher activity wastes. The process is used to demonstrate that the waste packages that would result from a proposal to package a particular waste will be passively safe and disposable, and in line with regulatory expectations for the long-term management of the waste [43].

The undertaking of each disposability assessment relies on a waste packager providing sufficient information regarding the waste, the proposed waste container and the waste conditioning processes to permit RWM to determine the expected properties of the waste packages that would be produced. This information is normally provided in the form of a packaging submission to RWM [44].

RWM produces an assessment report at the end of each stage in the Disposability Assessment process. The assessment report is intended to show in a transparent way

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10 Natural uranium contains 99.28% ^{238}U, with ^{235}U constituting about 0.71% by weight. Depleted uranium contains a lower content of ^{235}U than natural uranium. Low enriched uranium contains ^{235}U in a concentration of less than 20% and greater than 0.71% and highly enriched uranium contains anything between 20 and 100% ^{235}U.

11 DU stocks are mainly in the form of uranium hexafluoride (UF_6), a by-product of the uranium enrichment process used in the manufacture of nuclear fuels for AGR and PWR power stations. Current plans are for conversion of UF_6 into a less chemically reactive form more suitable for storage and disposal (U_3O_8). Significant quantities of DU are also stored as UO_3, the form arising from reprocessing of spent Magnox and AGR fuel.

whether the implementation of a packaging proposal would result in the production of waste packages that would be compliant with the relevant packaging specifications and the underlying safety, environmental and security assessments for transport and disposal. A Letter of Compliance (LoC) may be issued with the assessment report if we are satisfied that the implementation of the packaging proposal would result in the production of waste packages that are compliant with the relevant packaging specification and hence the geological disposal concepts and their associated safety cases.

The processes that a waste producer applies in order to ensure compliance with a stated fissile material limit (or any other criticality safety control) must be discussed and demonstrated in a Criticality Compliance and Assurance Document (CCAD), which forms part of the packaging submission. In discussion with RWM, a waste packager may derive a fissile mass limit specific to the proposed waste package or may use generic fissile mass limits derived by RWM, if applicable to the proposed waste package. The existence of, and compliance with, waste package fissile material limits is an assumption in the system-scale criticality safety assessments that form part of the DSSC.

Development of appropriate generic criticality safety controls, particularly fissile material limits, to support the Disposability Assessment process and the transport, operational and environmental safety cases is a key area of our research. The approach to derivation of safe fissile material limits is discussed in the following subsections.

3.3 Approach to deriving package fissile material limits

Criticality scenarios are defined and assessed in order to derive limits on the fissile material content of waste packages; limits are derived separately for transport, operations and post-closure scenarios.

This section discusses our approach to setting package fissile material limits and summarises the criticality scenarios considered for the transport and GDF operational and post-closure phases. The most restrictive fissile material limit calculated for these three distinct phases of the GDF lifecycle determines how much fissile material an individual waste package can contain.

Criticality scenarios are defined and assessed in order to derive limits on the fissile material content of waste packages. These limits ensure that the waste packages remain sub-critical when they are being transported to the GDF and during the GDF’s operational phase. Furthermore, these limits, along with parts of the GDF multiple barrier system, help to ensure criticality safety for a long period following facility closure.

Conditions during the transport and operational phases are more constrained and defined than in the post-closure phase as the GDF will continue to evolve over such long timescales. The approach to assessing criticality safety during the transport phase is also more prescriptive than for the operational phase. Therefore, whilst similar processes are assessed in all three phases, scenarios for each of the three phases are developed separately.

3.3.1 Package transport phase scenarios

Scenarios are defined to assess normal and accident conditions that may be experienced during waste package transport, for both single packages and package arrays. Regulations require that criticality is prevented during transport, so we apply a deterministic modelling approach.

The IAEA Transport Regulations [17] require that criticality is prevented during routine, normal and accident conditions of transport. The regulations strongly communicate a preference for engineered and passive safety measures (as opposed to operational / management controls) and specify the following events and processes that must be considered in transport criticality safety assessments:

- leakage of water into or out of packages
- loss of efficiency of built-in neutron absorbers or moderators
- rearrangement of the contents, either within the package or as a result of loss from the package
- reduction of spaces within or between packages
- packages becoming immersed in water or buried in snow
- temperature changes.

To address these requirements, criticality scenarios are defined that involve combinations of package design features, where these can be assured, and assumptions about package conditions that can be justified or can be shown to be pessimistic.

Typically, we specify transport phase accident scenarios that involve changes in package geometry, release of fissile material and water ingress. However, package designs may incorporate multiple water barriers, which must be demonstrated to remain watertight even under accident conditions and, in such cases, scenarios involving water ingress need not be evaluated. Consistent with the IAEA Transport Regulations [17], packages are assessed in isolation and in arrays of packages.

Assumptions about package behaviour during accident conditions are justified by, for example, the results of a combination of full-scale package drop tests and detailed finite element modelling analysis [7]. Where information about package material contents (such as geometric configuration, moderation properties and isotopic composition of fissile material) is uncertain or not known, a cautious approach is adopted in which parameters are assigned conservative values that maximise system reactivity.

3.3.2 GDF operational phase scenarios

Criticality scenarios assessed for operations are also based on consideration of normal and accident conditions. In a similar manner to that applied to the transport of packages to the GDF we also apply a deterministic modelling approach to the operational phase, although regulations do also permit a risk-informed approach should it be required.

Criticality scenarios assessed for the GDF operational phase are also based on consideration of normal and accident conditions. Again, scenarios are defined that involve justifiable assumptions about package design features and package conditions in their emplacement locations. Conditions that waste packages are subject to prior to, and for a short period after, buffer and/or backfill emplacement are considered under operational phase scenarios.

Typically, we specify scenarios that involve water ingress into waste packages after emplacement, although the GDF would be kept dry as far as possible during the operational phase prior to buffer and/or backfill emplacement. Such water ingress could occur if the waste packages have gas vents or are damaged. If the GDF concept involves emplacement of waste packages in arrays in, for example, a disposal vault, then we define scenarios in which the waste packages are closely packed, unless a minimum package separation distance can be assured. Known characteristics of the wasteform, such as the location of fissile and other materials in the waste package, may be included in the scenario assessment. However, where information about package material contents or operational phase conditions is not known, or is not demonstrable, parameters are assigned values that maximise system reactivity.

It is noted by RWM that paragraph 575 of the ONR Safety Assessment Principles (SAPs) [18] does allow for a risk-informed approach to operational criticality safety during the long-term storage of waste packages, an approach that balances the risks from an unplanned criticality accident against other factors, such as the dose accrued as a result of the preparation of waste packages. However, we believe that the first approach should be to pursue a deterministic argument in which controls are identified that will ensure criticality cannot occur during the operational phase. If this type of argument cannot be made for all waste packages (for example due to that fact that over batching[12] faults cannot be categorically ruled out), then options for a risk-informed approach will be considered.

3.3.3 GDF post-closure phase scenarios

Scenarios are considered which address post-closure physical and chemical processes that could result in for example, relocation, accumulation or concentration of fissile material over long periods of time, which could in turn possibly lead to a criticality.

Following closure of the GDF, physical and chemical processes could result in the relocation of fissile material over long periods of time. Such changes might reduce disposal system reactivity through dispersion of fissile material, but in some instances fissile material could accumulate, resulting in an increase in reactivity and the possibility of criticality if sufficient fissile material was to accumulate in an unfavourable arrangement. The events and processes that describe the evolution of conditions in a disposal facility after its closure are considered in the definition of post-closure criticality scenarios.

Post-closure criticality scenarios depend on the evolution of conditions in the near field of the GDF and the migration of fissile radionuclides over long time periods. The main processes considered in the identification of post-closure scenarios are:

- container degradation (for example, by corrosion) to the extent that water may enter or leave waste packages. Water may also move through container vents if present. Neutron moderation by the water may increase waste package reactivity.
- diffusion (and advection in the presence of flowing groundwater) of dissolved materials through degrading waste packages, surrounding buffer and backfill materials and host rock. Dissolution and loss of neutron-absorbing materials from a waste package could result in increases in package reactivity. The migration of fissile radionuclides in colloidal or particulate form, as well as in solution, may be significant, depending on material porosity and groundwater flow rates. The migration of fissile radionuclides may be influenced by the presence of organic complexants generated from components of the waste.
- collapse or compaction of waste packages following weakening by degradation or as a result of stress loading (such as rock fall or creep deformation of the host rock).
- gravitational settling or slumping of solid materials through voids created by the dissolution and removal of wasteform materials in groundwater. Solid fissile material and neutron reflecting materials (such as graphite) could relocate into configurations that result in increased system reactivity.
- sorption and precipitation of dissolved fissile radionuclides in the wasteform, engineered barrier materials and host rock, and filtration of fissile material in colloidal or particulate form. Precipitation could occur as a result of changes in the

[12] Over batching is a term used to explain a potential fault scenario where a waste package could inadvertently contains multiple loadings of fissile material and therefore breach the defined package safe fissile mass.

chemical environment akin to the formation of a mineral vein or seam in the geological environment. These processes could result in the accumulation of fissile material.

The above events and processes are considered in combination in order to define post-closure criticality scenarios for specific waste packaging and disposal concepts. Generally, scenarios are defined in terms of:

- those in which fissile and neutron moderating and reflecting materials relocate within a waste package such that system reactivity is conservatively assumed to increase for the resulting configuration
- those in which fissile material migrates from a waste package and accumulates elsewhere in the disposal system; such scenarios might involve accumulation of fissile material from single or multiple waste packages.

Detailed discussion of post-closure criticality scenarios is presented in Section 4, and in particular subsection 4.5.

The post-closure criticality scenario assessment timescales must take account of the time required for the evolution of conditions in the near field, radionuclide mobilisation and dispersion, and the radioactive decay of radionuclides of importance to criticality safety. For example, the fissile radionuclide ^{241}Pu has a half-life of 14.4 years and will decay to insignificant amounts before any post-closure criticality scenarios could be realised. The key fissile radionuclide ^{239}Pu has a half-life of 24,100 years; although ^{239}Pu decays to ^{235}U, which is also fissile, this results in a reduction in overall reactivity. However, ^{235}U has a very long half-life (704 million years) and its decay will be insignificant on the timescales of concern. We consider the occurrence of criticality scenarios on timescales of the order of tens to hundreds of thousands of years, based on cautious estimates of material degradation rates and groundwater flow conditions. For example, estimates of container corrosion rates are used to evaluate the earliest time at which water can enter a waste package and subsequent wasteform degradation and relocation processes can occur. Further discussion of post-closure criticality scenario assessment timescales is presented in subsection 4.4.

Historically, deterministic assessments of post-closure criticality scenarios have been undertaken which assume bounding pessimistic parameter values where there is any uncertainty. However, due to the increasing degree of uncertainty associated with waste package and GDF evolution over tens of thousands of years, deterministic post-closure assessments can lead to restrictive limits on fissile materials in a package, which in some cases could be considered to be inappropriate. Such limits may minimise the potential risk of post-closure criticality, but may also disproportionately increase the radiological and conventional safety risk to present-day workers. Therefore, recent research by RWM has focussed on developing probabilistic assessments of post-closure criticality scenarios, which apply probability distributions to parameter values to account for uncertainty and then appropriately sample these during assessment calculations. This research on the likelihood of criticality is discussed in Section 5 and parallel research considering the consequences of hypothetical post-closure criticality is discussed in Section 6. An alternative post-closure methodology for deriving less restrictive fissile material levels based on application of the likelihood and consequences of criticality research is discussed in subsection 3.4.3.

3.3.4 Derivation of waste package fissile material limits

Neutron transport codes are used to calculate the neutron multiplication factor to determine the limiting conditions for criticality for each of the transport, operational and post-closure phase scenarios. The most restrictive limit controls how much fissile material a waste producer can place in an individual waste package.

Criticality scenarios applicable to a particular waste package in the transport, GDF operational and post-closure phases are evaluated with the aim of determining the minimum conditions for criticality for a bounding quantity such as the fissile mass, concentration or enrichment. A suitable safety margin is then applied in order to set a safe fissile material limit for a waste package for each phase of waste management. The most restrictive limit from any of the three phases then controls how much fissile material a waste producer can place in an individual waste package.

The limiting conditions for criticality are usually determined using neutron transport codes, such as MONK [31] or MCNP [45], which are used to calculate the neutron multiplication factor $K_{effective}$ for the modelled system. The system is sub-critical if the calculated $K_{effective}$ is less than unity, but a safety margin is generally applied; typically, $K_{effective}$ is required to be less than 0.95. The modelling generally involves varying the mass and concentration of fissile material at a particular enrichment for each scenario, as well as the quantities of moderating and reflecting materials, until the minimum mass or concentration is found for which the specified $K_{effective}$ value is met. Waste package fissile material limits are then evaluated, taking into account scenario timescales (allowing for the decay of ^{239}Pu) and the number of waste packages that are judged to contribute fissile material to the model configuration.

Alternatively, limiting conditions for criticality may be obtained from criticality reference books (such as [46,47]) that provide information on critical masses and concentrations for a range of configurations and materials. Generally, a 20% safety margin is included if data from such reference books are used.

The application of this approach to deriving waste package fissile material limits is described in the following subsections: ILW and LLW packages (subsection 3.4); HLW and SF packages (subsection 3.5); and DNLEU, HEU and plutonium packages (subsection 3.6).

3.4 ILW/LLW and DNLEU package fissile material limits

A hierarchy of package fissile limits for ILW, LLW and DNLEU are calculated, based on assumptions concerning the packaging and wasteform. Additional considerations are taken into account for post-closure scenarios to ensure a sufficiently risk-informed approach is taken for the derivation of the overall package limit.

We begin this section by summarising the range of wasteforms and containers that may be used for ILW/LLW and DNLEU. We then outline the hierarchy of ILW/LLW and DNLEU (collectively referred to as low heat generating waste (LHGW)) package fissile material limits for package transport, and the GDF's operational and post-closure phases. Recent work to extend our process for establishing post-closure fissile material limits for LHGW packages is then summarised.

3.4.1 Packaging and wasteform assumptions

A range of standard containers are available that are suitable for packaging the majority of the ILW and LLW inventory, although waste producers may propose additional containers. Cementitious grout is generally used to encapsulate the majority of the waste.

Encapsulation with cementitious grout has generally been used to condition ILW and LLW. However, alternative immobilisation and encapsulation matrices, such as glass, ceramics and polymers, may be more suitable for ensuring long-term containment of certain types of waste under disposal conditions. In addition, some waste types may not be immobilised at all, depending on the properties of the waste and the waste container to be used.

RWM has defined a range of containers that are considered suitable for packaging the majority of the ILW and LLW, although waste producers may propose additional containers. The standardised containers include 500 litre drums, 3 m^3 boxes, 3 m^3 drums, 6 m^3 boxes, and 2 m and 4 m boxes, as well as a range of robust shielded containers (RSCs; thick-walled containers that provide a high degree of waste containment and package performance).

Figure 3 provides illustrations of a selection of RWM’s standardised containers.

Figure 3 Examples of possible ILW/LLW containers (a) the 500 litre drum. (b) the 3 m^3 box

The development of a packaging concept for uranium wastes is at an early stage. For the preparation of the Derived Inventory for uranium [39], DNLEU was assumed to be packaged as U_3O_8 and mixed with a grout encapsulant in 500 litre drums and treated as ILW. A research project has recently considered alternative disposal options for DNLEU. The project concluded that, at least for the depleted and natural uranium component, disposal of larger waste containers of non-immobilised uranium in its current storage form was feasible and preferable [48]. As part of this work, a scoping level criticality safety assessment of proposed options for LEU disposal was also conducted which focused on possible criticality control options for LEU packaging [49]. Nonetheless, the safety assessments discussed below for low heat generating waste (LLW, ILW and DNLEU) were undertaken using the original assumption of DNLEU encapsulated in 500 litre drums.

3.4.2 Hierarchy of fissile material limits

We use a hierarchy of fissile material limits for ILW. As one moves up the hierarchy, credit is taken for increasing knowledge of the specific waste stream and its characteristics.

RWM's research in support of waste package criticality safety has focussed on ILW and LLW packages and this has led to the derivation of a hierarchy of fissile material limits for ILW/LLW and some DNLEU packages. As one moves up the hierarchy, credit is taken for increasing knowledge of the specific waste stream, and its characteristics, in deriving fissile material limits. Packaging to these increased fissile material limits can only be justified if there is a demonstration of the waste package understanding necessary to ensure compliance with requirements on package criticality controls.

The first level is a general screening level (GSL) of 50 g ^{239}Pu (or its equivalent). The general criticality safety assessment (GCSA) [50] is based on wastes being packaged with limits on the content of graphite (1 kg), beryllium and deuterium (both 100 g); a slightly lower fissile material limit applies if an unlimited amount of graphite is possible. Package-scale scenarios have been defined to cover the operational and post-closure periods. These package-scale scenarios were deterministically calculated assuming optimum (in terms of achieving criticality) geometries and concentrations for the accumulation and interaction of pure fissile materials, resulting in a very robust GSL that can be applied to waste packages containing any fissile radionuclides.

The next level is represented by the generic Criticality Safety Assessments (gCSAs). Four have been produced for common categories of fissile ILW packaged in 500 litre drums, 3 m^3 boxes and 3 m^3 drums: highly enriched uranium [51], low-enriched uranium [52], irradiated natural uranium [53] and separated plutonium [54]. The gCSAs recognise generically (to ensure wide coverage) the isotopic variations of uranium and plutonium, which results in significantly higher fissile material limits for packages containing natural and low-enriched uranium wastes. A fifth gCSA [27] has also been produced for irradiated natural and low-enriched uranium packaged in RSCs.

The gCSAs deterministically derive limits for transport, operations and the post-closure phase, although the RSC gCSA [27] does not include a quantitative assessment of the waste package transport phase because the transport arrangements for RSCs have not yet been defined at a generic container level. The first four gCSAs include a set of indicative fissile material limits, from the relevant Package Design Safety Report [55], which are deemed to be consistent with the requirements of the IAEA Transport Regulations [17]. In most cases, the transport phase fissile material limits are more restrictive than the operationally-derived fissile material limits, which is unsurprising given the prescriptive and conservative nature of the IAEA Transport Regulations.

At the time that the first four gCSAs were being developed, the band methodology [56] was being developed between the regulator and site operators to derive package 'limits' for interim storage. It was subsequently agreed with the regulators that the principles of the band methodology would be applied in the GDF operational phase. To reflect this, and recommendations from regulatory scrutiny [57], the gCSAs introduced lower and upper screening levels in the GDF operational and post-closure phase assessments. The treatment of these phases in the gCSAs is therefore based on the derivation of two 'screening levels': a Lower Screening Level (LSL) intended to represent a highly conservative view of possible scenarios and an Upper Screening Level (USL) that adopts a more credible, yet still conservative representation.

The screening level approach is based on the fact that the composition and characteristics of the waste package are inherently controllable through measures such as the design of that package, application of suitable characterisation and the operation of the packaging process. Typically, the better a package can be controlled, the more the conservatisms in the description can be reduced, leading to a higher screening level. Consequently, the USL values are based on more specific descriptions of the packages, as far as is possible within a generic criticality safety assessment. An increased fissile material limit does not imply increased likelihood of criticality, but rather reflects better (substantiated) knowledge of the waste package.

The final level in the hierarchy of fissile limits provides for package-specific criticality safety assessments which take account of additional information about the waste or package to justify an increased fissile material limit. This would normally require specific information on the geometry and isotopic concentrations of fissile materials and on the presence and persistence of any neutron absorbing materials.

The hierarchy of fissile limits for waste packages, from the GSCA to the relevant gCSA and then to a package-specific limit, is illustrated in Figure 4. Note, package specific limits will not necessarily always be greater than the GCSA or gCSA derived limits.

Figure 4 Hierarchy of fissile material limits for waste packages

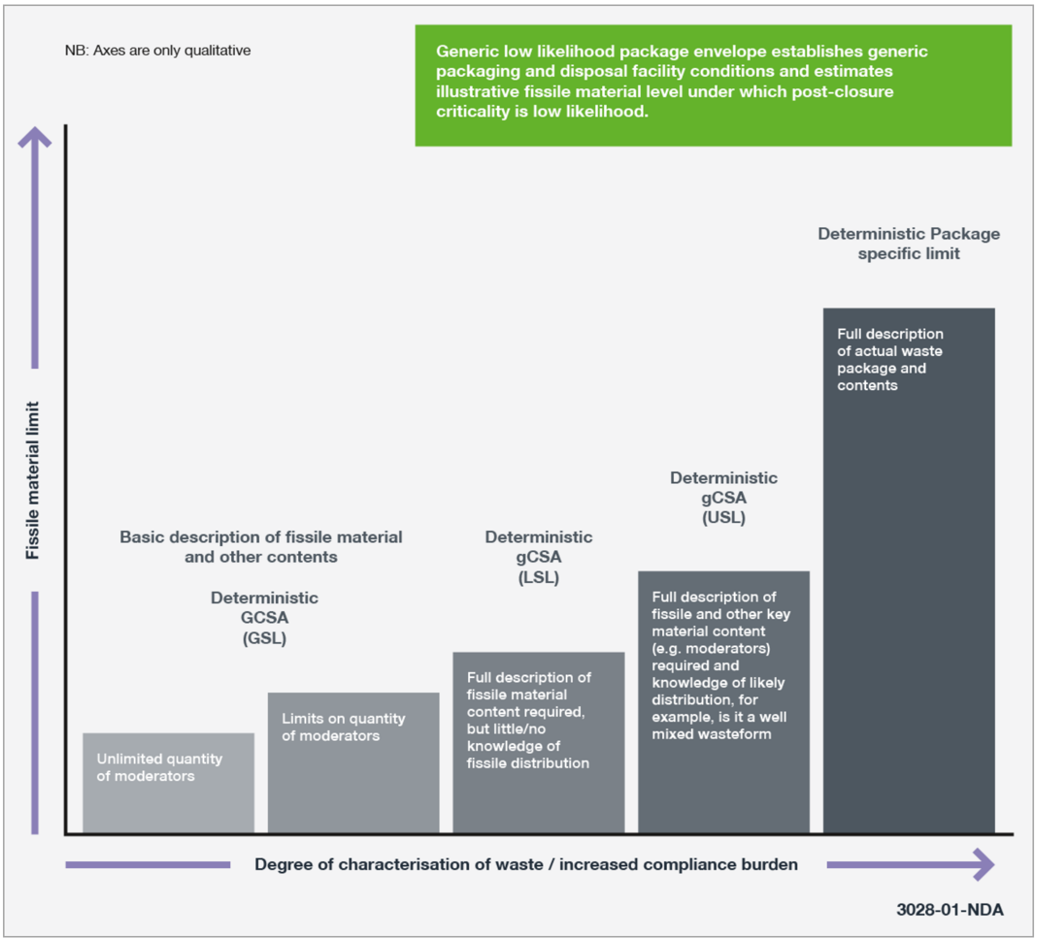


Figure 4 also introduces the idea (see the green box) that post-closure fissile material limits can be estimated using not only a deterministic approach, but also using a probabilistic approach. This probabilistic approach is only relevant to the post-closure phase of the GDF lifecycle and only when arguments to demonstrate low consequences of post-closure criticality can be applied, as discussed in subsection 3.4.3 in the context of a generic low likelihood package envelope.

3.4.3 Package envelope approach for post-closure criticality safety assessment

Placing limits on fissile material in packages based on highly stylised conservative post-closure scenarios can lead to very restrictive limits. If it can be shown that a packaging proposal is consistent with research that shows the likelihood of post-closure criticality is low, packaging to a higher probabilistically (as opposed to deterministically) derived limit can be justified.

To date, the basis for ensuring criticality safety of LHGW has been to control the maximum fissile material content of individual packages via deterministic assessments using bounding pessimistic parameter values. In practice this approach, whilst ensuring post-closure criticality safety, results in restrictive limits that are derived using highly stylised and overly conservative post-closure scenarios occurring at very long timescales into the future. RWM, the industry and the regulators do not consider this approach to yield an appropriate balance of risk between current waste processing operations and the distant future.

Therefore, our recent research has focussed on developing probabilistic assessments of post-closure criticality scenarios. This has led to the proposal of a generic 'low-likelihood package envelope' that establishes the packaging and disposal facility conditions under which post-closure criticality is considered unlikely to occur. A detailed account of this work is reported in [58]. If waste producers can demonstrate adherence to this package envelope then no further post-closure criticality safety assessment is required and increased individual package fissile material loadings are possible. We anticipate that application of this methodology will mean that, in general, the existing deterministic transport limits will be bounding in most cases. This 'package envelope' approach provides an alternative option for those packages that meet the envelope criteria.

The package envelope encompasses most LHGW (ILW, LLW and DNLEU) that is grouted into 500 litre drums, 3 m^3 boxes or 3 m^3 drums. The wider methodology (also explained within [58]) requires that arguments to demonstrate low consequences of post-closure criticality should also always be applied.

The approach to defining the generic low-likelihood package envelope essentially represents an extension of the deterministic approach currently used in criticality safety assessments to derive waste package fissile material limits. However, rather than making worst case assumptions about parameter values with regard to the likelihood of criticality, a probabilistic approach has been taken in which waste package degradation and the relocation of fissile and other materials have been modelled. Bounding parameter values have been identified for which the minimum conditions for criticality are not achieved during a one million year assessment timeframe for any of 1,000 probabilistic calculations undertaken. That is, even accounting for extreme combinations of low probability parameter values captured in parameter value sampling, waste package evolution and the migration and relocation of fissile material would not result in criticality; this condition defines the target value assumed for demonstrating low likelihood of criticality.

The parameters that define the package envelope are summarised in Table 2. Assumptions about the host rock and engineered barrier system characteristics and how they influence waste package evolution are important components of the package envelope definition. In this work, evaluation of the package envelope was based on RWM's illustrative concept for the disposal of LHGW in vaults in higher strength rock and assumptions about system evolution consistent with those made in the Likelihood of Criticality project. The assumed conditions bound those expected for disposal in lower strength sedimentary rock and evaporite in terms of the analysis of the likelihood of post-closure criticality, based on the illustrative disposal concepts for such host rocks presented in the Technical Background Document of the generic DSSC [1].

Table 2 Summary of bounding package envelope parameters for LHGW [58]

Component	Parameter
Waste package characteristics	The waste is packaged in a stainless steel container: • 500 litre drum • 3 m^3 box • 3 m^3 drum. The wastes may contain the fissile radionuclides ^{239}Pu and/or ^{235}U (calculated as an equivalence[13]), up to the derived fissile material limit. Other fissile radionuclides can only be present in insignificant amounts (gram quantities). Credit may be taken for the presence of ^{238}U in the waste, which acts to dilute the fissile material and to absorb neutrons. The wastes are encapsulated and mixed with cementitious grout in the containers. The wastes do not include materials that could preferentially accumulate fissile radionuclides (such as a material that has a greater capacity for sorption of uranium and plutonium than the backfill) [5].
Waste package performance under disposal conditions	Waste package behaviour under disposal conditions is captured by the parameter value distributions adopted in the modelling analysis. Assumptions about waste package behaviour under disposal conditions are: • container corrosion rates in the range 10^{-5} to 10 µm/yr • plutonium solubility limits in the range 10^{-8} to 10^{-5} mol/m^3 • uranium solubility limits in the range 10^{-8} to 10 mol/m^3 • grout persists in the waste package such that gravitational slumping does not occur on a timescale of 1.3×10^5 years.
GDF conditions	The conditions assumed in the illustrative disposal concept for the disposal of LHGW in vaults in higher strength rock bound the conditions in any future GDF. These conditions are primarily captured by parameter value distributions for groundwater flow through the vaults, and uranium and plutonium sorption distribution coefficients for the backfill.

In the Likelihood of Criticality research project, it was not possible to demonstrate that the likelihood of post-closure criticality from a small proportion of LHGW packages would be zero (based on the consideration of waste package evolution under disposal conditions) without imposing limits on the fissile material contents of waste packages. Therefore, we have identified limits on the fissile material contents of LHGW packages that will ensure that post-closure criticality is unlikely to occur[14], based on the models used and parameter value distributions adopted in the Likelihood of Criticality research project. That is, maximum fissile masses have been evaluated for which the target value assumed for the likelihood of criticality is met.

13 For example, by considering their contribution to reactivity in terms of ^{239}Pu equivalence.

14 In the low likelihood package envelope approach, criticality is judged to be of 'low likelihood' if none of 1000 probabilistic model runs results in the accumulation of a minimum critical mass or concentration over a one million year duration.

Note that a cautious deterministic approach has been taken with regard to the assumed geometry of the accumulated material at different locations in the GDF after closure (hence, worst case spherical and infinite slab geometries have been assumed). Conditions at which the calculated neutron multiplication factor remains below unity for these assumed configurations have been sought. This differs from the cautious deterministic approach historically used to derive post-closure fissile material limits on waste packages, where a safety margin is adopted on the neutron multiplication factor. The reason for this difference in approach and the other main differences between the probabilistic modelling analysis and the deterministic analyses are listed in Table 3.

Table 3 Key differences between the deterministic analysis and the probabilistic analysis for calculating maximum waste package fissile material limits [58]

Key aspect	Deterministic analysis	Probabilistic analysis
Post-closure criticality safety criterion	Demonstrates that post-closure criticality cannot occur (for the scenarios considered) through deterministic analysis of criticality scenarios, based on a worst-case treatment of uncertainty. The maximum mass of fissile material in a waste package is controlled such that criticality cannot occur for any of the scenarios assessed.	Uses a defined low-likelihood criterion to demonstrate post-closure criticality safety based on a probabilistic treatment of uncertainty in scenario analysis. The maximum mass of fissile material in a waste package is controlled such that criticality does not occur over a one million year duration for any of 1,000 probabilistic model runs.
Scenarios assessed to derive limits	Limits derived from the most restrictive of: **Single 'package-scale' analysis**, which considers slumping of fissile material in the package. **Multiple package 'stack-scale' analysis**, which considers slumping of fissile material through a seven-high stack of packages. Fissile material accumulation in the backfill surrounding the waste packages was not modelled; fissile material from a maximum of seven packages could contribute to an accumulation.	Limits derived from the most restrictive of a more detailed analysis, including: **Single package analysis**, which considers accumulation by slumping of fissile material in the package and accumulation by advection of fissile material and sorption in the backfill. **Multiple package analysis**, which considers the release, migration and mixing of fissile material from many waste packages in a disposal vault, including the slumping of fissile material through seven-high stacks of degrading waste packages.
Timescales for package and stack slumping	In defining the limit, slumping of a single package is assumed to occur after 15,000 years. Slumping through a stack of seven waste packages is assumed to occur after 60,000 years.	The timing of slumping in each waste package depends on the volume of water required to dissolve waste package grout and the flow rate through the degrading waste package, which are sampled parameters in the probabilistic analysis. It would take some 260,000 years to dissolve and remove 500 kg of grout from a 500 litre drum in the unlikely event that the package was exposed to

Key aspect	Deterministic analysis	Probabilistic analysis
		water that has not been conditioned to high pH by the cementitious backfill and that it is flowing at the highest assumed rate through the waste package[15].
Assumed geometries of fissile material accumulations	A slumped system is represented by a water-moderated, water-reflected sphere in the lower screening level calculations and a water-moderated, water-reflected slab in the upper screening level calculations.	A slumped system is represented by a water-moderated, water-reflected slab. An accumulation in backfill is represented by a water-moderated, water-reflected sphere.
Criticality safety margins	Calculation of waste package fissile material limits based on analysis of post-closure scenarios included an arbitrary 5% safety margin on the neutron multiplication factor.	No safety margin is included on the neutron multiplication factor when evaluating waste package fissile material limits. The probabilistic modelling approach enables parameter value uncertainty in post-closure scenarios to be accounted for by randomly sampling parameter value probability distributions (that contain built in conservatisms) over many realisations. There is therefore no need to add an additional arbitrary safety margin to account for parameter uncertainty. Also, a criticality event after GDF closure would not pose an immediate and direct risk to workers or members of the public and, therefore, an arbitrary safety margin is unnecessary. Furthermore, the risks associated with a hypothetical criticality event in the GDF have been addressed separately in our GDF post-closure criticality consequences assessment in order to support demonstration in the environmental safety case that the regulatory risk guidance level is met.

15 500 kg of wasteform grout is assumed to be contained within a 500 litre drum. We arbitrarily assume that 50% of this grout needs to be removed to allow package slumping to occur. The low likelihood package envelope work has shown that it would take in excess of 130,000 years for this mass of grout to be removed.

3.4.4 Post-closure criticality safety assessment methodology

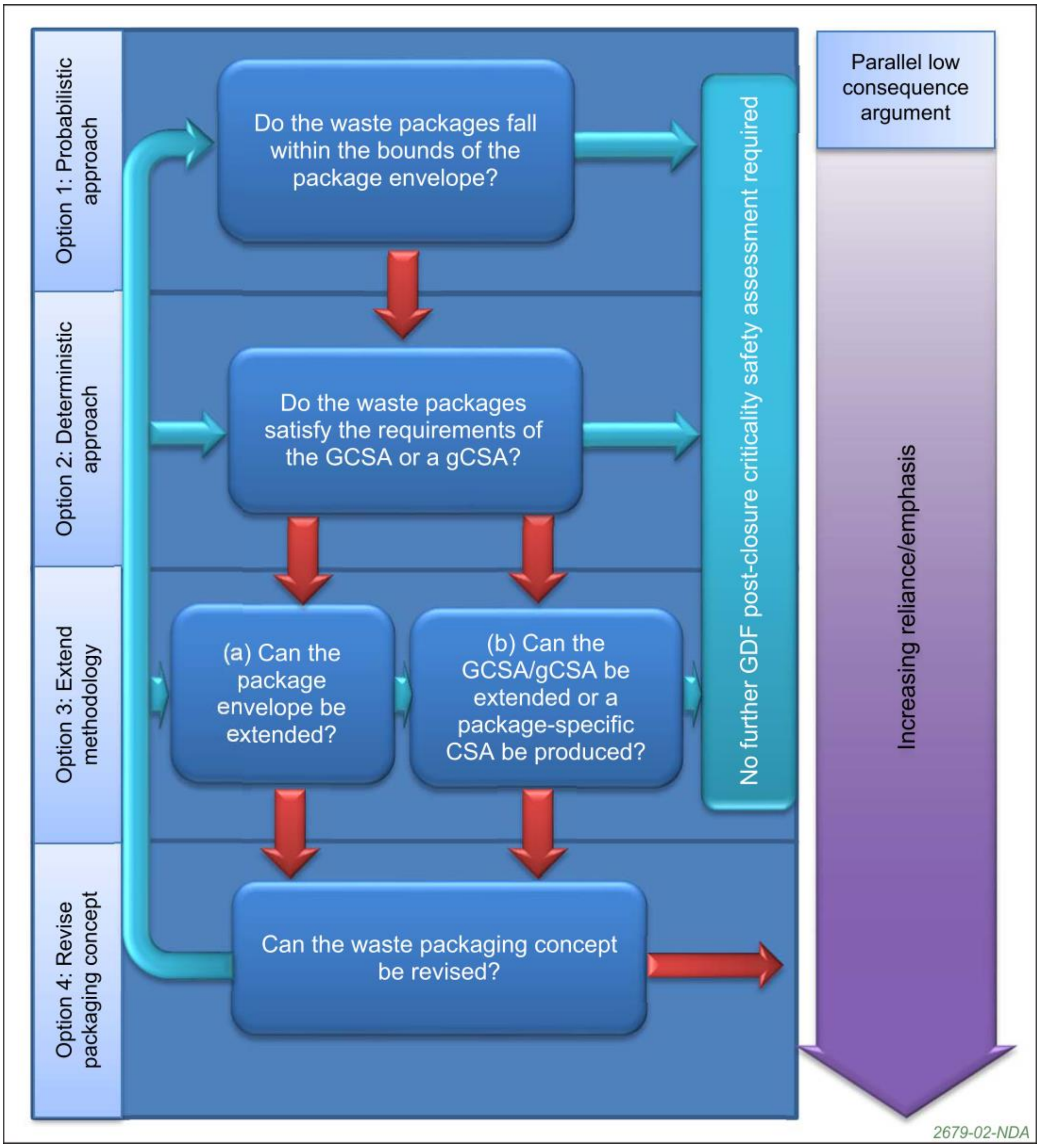
The most restrictive deterministically derived fissile material limit from the transport, operational or post-closure phase assessments controls how much fissile material a waste producer can place in an individual waste package, unless waste package characteristics are consistent with a post-closure 'low likelihood package envelope'. In this case the next most restrictive deterministically derived fissile material limit (be it from the transport or the operational phase) should be used to control package fissile material content.

Our methodology for ensuring post-closure criticality safety of all LHGW packages has been developed to enable waste producers to take advantage of the package envelope analysis.

This approach is not inherently new, but the enhanced knowledge base (see Sections 5 and 6) has provided more robust underpinning and also developed and facilitated better communication of our existing position with regard to low consequences. Furthermore, as discussed in subsection 3.4.3, the package envelope option has been introduced to offer more flexibility to waste producers with regards to demonstrating low likelihood compliance.

The parallel low consequence strand of the argument (see the right-hand side of Figure 5) should always be applicable to disposability assessments, but becomes increasingly important the more a post-closure criticality safety assessment relies on the long-term performance of a container or wasteform characteristic in order to make a low-likelihood argument (that is, the further it moves away from a traditional deterministic approach, the greater the uncertainty in that argument becomes). As the uncertainty increases our methodology requires an increased reliance on the understanding and demonstration of low consequences.

Figure 5 Flow-chart for post-closure criticality safety assessment methodology. A blue arrow indicates "yes" and a red arrow indicates "no" [58]



The different options in the methodology for ensuring post-closure criticality safety of all LHGW packages are as follows:

Option 1: Comparison with package envelope criteria

The first option in the methodology involves determining whether a waste package falls within the bounds of the generic low-likelihood package envelope, as defined in Table 2 and Table 3. Note that, hereafter, the bounds of the package envelope are referred to as 'envelope criteria'.

Option 2: Comparison with the requirements of the GCSA or a gCSA

If a waste package does not meet the envelope criteria because, for example, an encapsulating grout is not used, or a container different from those listed in Table 2 is proposed, then it may be possible to show that the package is acceptable for disposal based on consideration of the requirements derived deterministically in the GCSA or an appropriate gCSA.

Option 3: Extension of the methodology

If waste package criticality safety cannot be demonstrated using either of the above options (meaning that the waste package does not satisfy the envelope criteria or the requirements of the GCSA or a gCSA), then it may be possible to extend the methodology to address the packaging concept in question according to Option 3a or Option 3b.

Option 3a: Extension of the package envelope

Extension of the package envelope could involve showing that, although the waste package does not meet all of the envelope criteria, its behaviour under disposal conditions is bounded (from a criticality safety perspective) by assumptions made about package behaviour in the analysis to derive the envelope criteria. For example, an alternative waste container and/or waste encapsulation/immobilisation matrix may be proposed, but it may be possible to demonstrate that the proposed waste package is at least as durable under disposal conditions as the grouted waste packages assumed in the analysis to derive the envelope criteria. Such a demonstration would imply that post-closure criticality is no more likely to occur for the proposed waste package than for the waste packages covered by the package envelope. Alternatively, if such bounding arguments cannot be made, the models used in the analysis to derive the package envelope could be modified to include the proposed waste package, such that probabilistic calculations could be undertaken to revise the envelope criteria.

Option 3b: Extension of the GCSA or a gCSA or production of a package-specific CSA

Option 3b involves either demonstrating that the waste package is bounded by assumptions made in the GCSA or a gCSA in terms of wasteform composition and waste package durability under GDF post-closure conditions (even if the package does not directly meet all of the GCSA or a gCSA requirements), or producing a deterministic package-specific CSA. The latter may involve revising an existing gCSA to cover, for example, a variation in container properties or in uranium enrichment, or taking credit for a specific waste package characteristic (such as a diluent or neutron absorbing material that could be shown to persist in the waste package).

Option 4: Revision of the waste packaging concept

An alternative approach would be to modify the waste packaging concept to achieve compliance with the envelope criteria or the requirements of the GCSA or a particular gCSA. However, such an approach may involve operations that expose workers to radiological risks deemed to be excessive in comparison with the potential risks of post-closure criticality in the GDF. That is, the approach may not satisfy the holistic principle of ensuring that risks are ALARP [18].

If revision of the waste packaging concept is not ALARP then, on a case-by-case basis, and only for specific, low quantity, high fissile-content waste packages, it may be possible to consider a special emplacement strategy in the GDF. Selective emplacement of relatively high fissile-content waste packages (and control of the fissile material loading of waste packages stacked with such packages in a vault) is an option that can be used to achieve a relaxation of package fissile material limits derived from consideration of post-closure stack slumping scenarios. However, this is not a default option, nor a method to avoid restrictive post-closure safe fissile material limits, and may only be available for a small number of waste streams after it has been clearly demonstrated that all alternative options have been explored and would not be ALARP.

Parallel low consequence argument

Low-consequence arguments should always be applicable to disposability assessments, but increased reliance on such arguments should only be pursued if satisfactory probabilistic or deterministic arguments cannot be made to demonstrate post-closure criticality safety (Options 1 to 3), and modifications to the packaging concept would introduce unacceptable risk (Option 4). Furthermore, this increased reliance on low-consequences arguments is only considered acceptable if it can be demonstrated (through Options 1, 2 or 3) that disposal of the proposed waste packages would not lead to rapid transient criticality. That is, a low consequence argument would only be acceptable for possible quasi-steady-state criticality events.

Summary

It is expected that the post-closure criticality safety of the vast majority of LHGW packages could be demonstrated using Options 1 or 2 of the methodology, as discussed above. Of course, criticality safety requirements associated with waste package transport and GDF operations also need to be considered in a full waste packaging assessment. Hence, waste package safe fissile masses should be identified using the screening level methodology discussed in subsection 3.4.2 and set out in [41] for waste package transport and the GDF's operational phase, and the constraints imposed by application of the methodology presented here for the post-closure phase.

3.5 HLW and SF package fissile material limits

Spent fuel contains significant quantities of fissile material, while HLW contains small amounts of fissile material; the average fissile content in a HLW container is expected to be only ~45 g ^{239}Pu and ~5 g ^{235}U, which does not represent a criticality safety concern.

In this section we discuss the HLW and SF wasteforms and disposal containers that may be used. Unlike for much of the ILW inventory, we will possess detailed records regarding the exact package content for the majority of SF requiring disposal. Furthermore, the wasteform design is already fixed and the majority would be considered to be relatively corrosion resistant (for example, a ceramic fissile material surrounded by Zircaloy or stainless steel cladding).

In contrast to SF, HLW only contains small amounts of fissile material, which is immobilised in a stable borosilicate glass wasteform. As discussed in subsection 3.1, the average fissile content in a HLW container is expected to be only ~45 g ^{239}Pu and ~5 g ^{235}U, which does not represent a criticality concern. Also, it is expected that controls on the physical and chemical form of HLW will ensure that variations in the fissile material content of HLW packages are relatively small, such that to assume average values for HLW package contents is reasonable.

3.5.1 Packaging and wasteform assumptions

No decisions have yet been made on the packaging of HLW or spent fuel for disposal as the disposal system design will be site-specific. For assessment purposes, packaging assumptions have been made based on our three illustrative geological disposal concepts.

Spent fuel is likely to contain much higher concentrations and masses of fissile radionuclides than those typically found in ILW. As previously discussed, the majority of ILW packages will be designed to be sub-critical by limiting the fissile radionuclide mass, concentration and/or enrichment in each package, but this is not feasible for SF. Therefore, we will rely on the design of the package for SF, as well as the wasteform, to ensure criticality safety. As future SF CSAs are expected to make use of specific knowledge about the content of each package, the wasteform and the package design, package-specific CSAs will be developed (equivalent to the final level in the LHGW fissile material limit hierarchy of Figure 4).

The final packaging concept for HLW and SF disposal has not yet been decided but, for assessment purposes, packaging assumptions have been made based on our three illustrative disposal concepts. A description of our illustrative disposal concepts and packaging assumptions is given in [1], although to aid understanding a brief summary of the packaging assumptions for HLW and SF is given below.

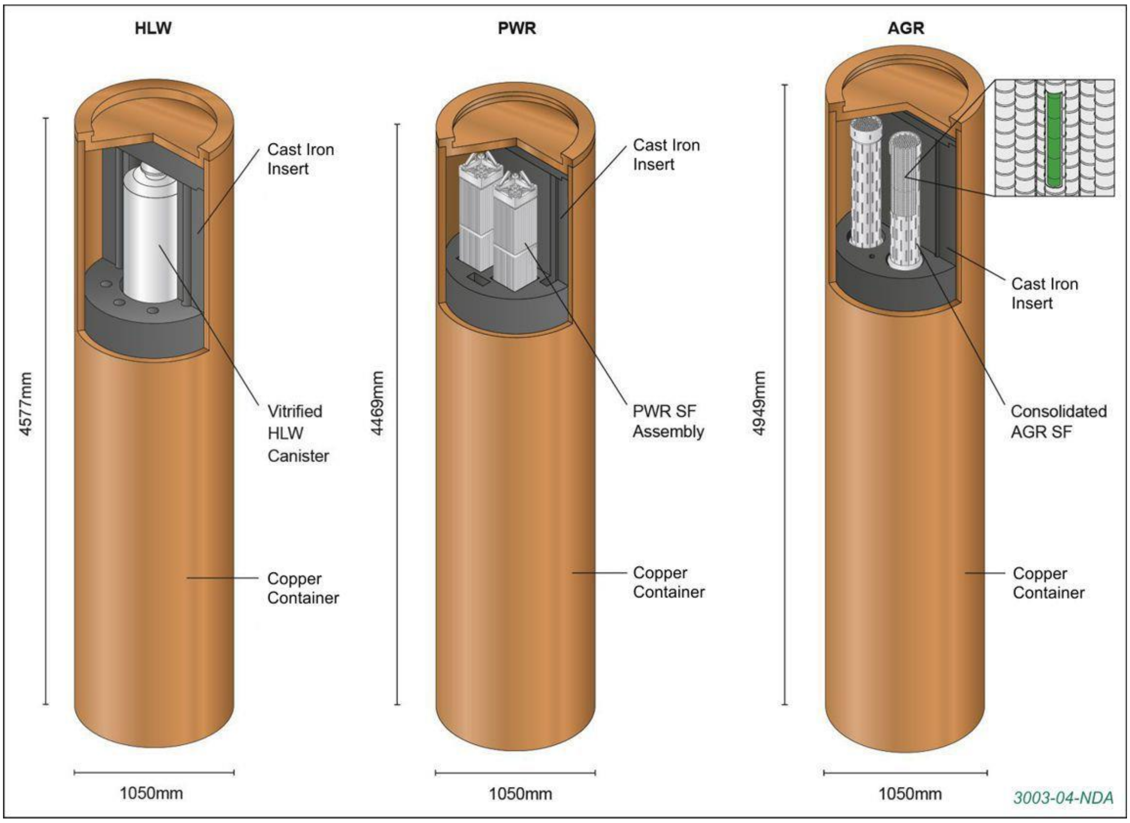
For the illustrative concept for higher strength rock, it is assumed that the disposal container will be a welded 50 mm thick copper shell, with structural integrity provided by an internal cast iron insert (see Figure 6). For the illustrative concepts designed for lower strength sedimentary rock and evaporite it is assumed that the disposal container will be based on a carbon steel container design.

A set of concept designs for three different disposal containers (to contain legacy HLW and PWR and AGR SF) has been developed for the UK and has recently been optimised and rationalised [59]. Comparable designs for new build and MOX SF are not yet available, but are envisaged to be similar. The following assumptions have been made:

- HLW – three HLW canisters will be stacked in each disposal container (as shown in Figure 6).
- PWR SF – four PWR fuel assemblies will be packaged whole within a single disposal container (as shown in Figure 6).
- AGR SF – AGR fuel assemblies will be dismantled prior to disposal, with graphite removed and the fuel pins consolidated into bundles and placed in slotted cans. A total of sixteen consolidated fuel bundles (equivalent to the pins from 48 AGR elements) will be packaged inside a disposal container (as shown in Figure 6).
- new build SF – SF from AP1000 and UK EPR reactors is assumed to be similar in size and is, therefore, considered together. Three new-build fuel assemblies (assumed to be at 65 GWd/tU burn-up) will be packaged whole within a single disposal container[16].
- MOX SF – MOX SF is assumed to be packaged whole, but with only one fuel assembly in a disposal container (primarily due to its higher thermal output).

[16] Potential new build Boiling Water Reactor (BWR) spent fuel is also likely to be packaged for disposal in this way, although it is not specifically identified in the 2013 Derived Inventory.

Figure 6 The copper and cast iron disposal container design, assumed for a higher strength rock geology, showing the three internal configurations used for disposal of HLW (left), PWR SF (centre) and AGR SF (right). A carbon steel variant would be used for the lower strength sedimentary rock and evaporite geologies.



Whilst the above packaging assumptions have been made, the packaging design for HLW and SF is not final. Further criticality safety assessment work will shortly be undertaken on the UK disposal container design, see [10] tasks 69, 74 and 78. Furthermore, research is also currently being undertaken on alternative disposal concepts, such as the possibility of using multi-purpose containers (MPCs) for PWR SF management [60] (see [10] task 66). Finally the development of alternative wasteforms for MOX fuel disposal is also an area of ongoing work, which is being led by the Nuclear Decommissioning Authority in order to support Government policy in this area.

3.5.2 Criticality safety research

It is not feasible to ensure sub-criticality by limiting the fissile mass in a spent-fuel package. Instead, the package and wasteform can be designed such that it remains sub-critical.

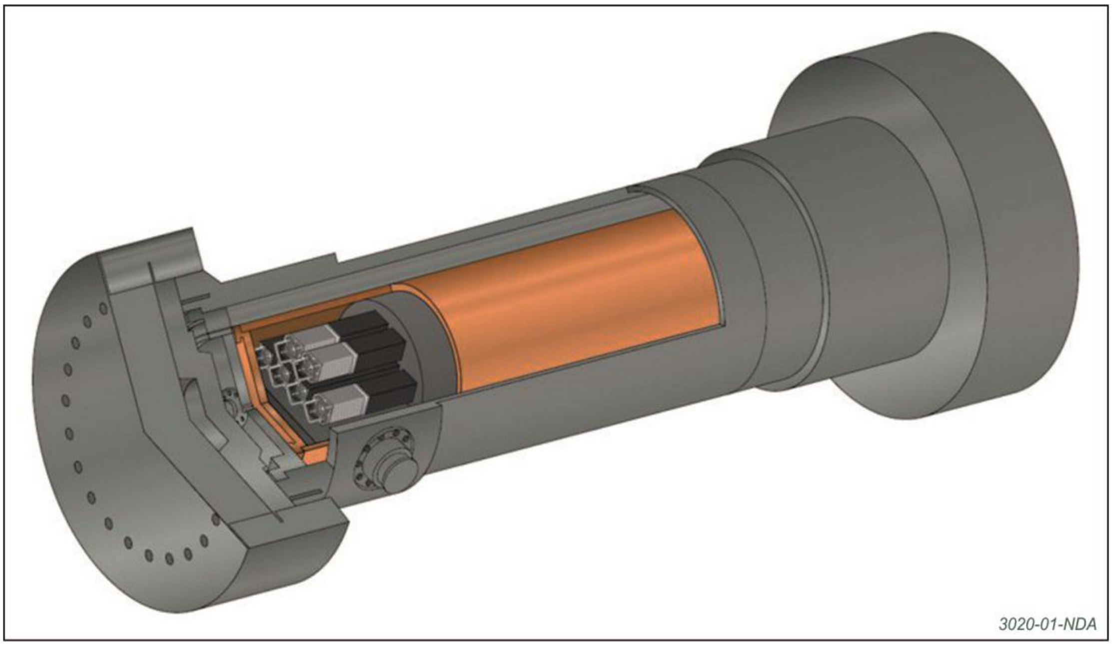
As potential disposal packages are at such an early illustrative stage, no fissile controls have been developed by RWM for SF. However, it is anticipated that, based on criticality assessments undertaken for SF disposal in Sweden (upon which the copper disposal container design is based), the UK designs for most SF disposal containers will include substantial criticality safety margins. Long-term criticality safety relies on the isotopic composition of the fuel and the stable long-lasting form of the waste matrix and its waste container.

RWM recently examined possible DCTC design configurations for compliance with the criticality safety requirements of the IAEA Transport Regulations [17]. One package design feature that is being explored by RWM to ensure SF packages remain sub-critical is the use of a high integrity package that has multiple high standard water barriers[17]. An options study [26] determined that the preferred criticality safety solution for transport of SF in the public domain is to use a transport package with multiple water barriers. Such a transport container would ensure that significant water ingress is excluded under challenging accident conditions that require the assumption that at least one containment barrier has failed during an accident scenario. Therefore, using multiple water barriers ensures that even if one containment barrier were to fail, water can still not access the container contents and increase system reactivity.

Another possible option is the inclusion of neutron poisons in the package (see [10], tasks 68 and 69), although their persistence during transport and operational accident conditions, and during post-closure package degradation, will need to be demonstrated.

There is extensive UK and international experience of transporting SF. Generally, SF transport makes use of transport containers (often referred to as 'flasks') that are specific to the reactor type (for example, PWR, AGR or Magnox reactors). Our current design assumption is that SF will be transported to the GDF in its disposal container inside a Disposal Container Transport Container (DCTC), a conceptual illustration of which is shown in Figure 7. The exact design is still being developed (see [10] tasks 80 and 81).

Figure 7 Conceptual illustration of a DCTC, shown on its transport and handling frame, and holding a copper disposal container



HLW and SF disposal containers will be removed from their transport container (the DCTC) once they are received at the GDF. This means that an argument based on the use of multiple water barriers in the transport phase may not be directly transferable to the GDF's operational phase. Therefore, alternative criticality control measures may be required or a double contingency approach[18] may need to be used.

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17 Multiple water barriers - see IAEA Transport Regulations [16], subparagraph 680.

18 A double contingency approach involves a demonstration that unintended criticality cannot occur unless at least two unlikely, independent, concurrent changes in the conditions originally specified as essential to criticality safety have occurred [18].

Criticality safety assessments typically assume that the fissile material is in its most reactive condition, which is usually at maximum enrichment with no irradiation. Fission products and actinides are formed during irradiation of the fuel in the reactor, a process which also tends to reduce the overall concentration of fissile material. Accounting for the resulting reduction in reactivity is known as ‘burn-up credit’ and can provide significant increases in derived safe fissile material limits [61]. Use of burn-up credit arguments is an area of future research for RWM (see [10], tasks 73, 77 and 79), although such arguments require a detailed record of the SF irradiation history and a significant management control. Such an assurance burden may not always be possible for all SF.

Application of burn-up credit to disposal operations is very limited in the UK and, indeed, world-wide. However, studies on the application of burn-up credit to disposal operations have been made, notably in the USA and Sweden [62, 63], which provide a useful starting point for similar studies for UK disposal plans (see [10] tasks 68, 73, 77 and 79). Belgian studies on the disposal of SF have included assessing the potential for forming a critical system through re-arrangement of material within a package following closure [64]. The likelihood of post-closure criticality safety work discussed in Section 5 takes credit for the irradiation history of SF, meaning that it utilises burn-up credit to support a generic demonstration of the safe disposal of SF. In addition, the parallel consequences of hypothetical post-closure criticality work (see Section 6, particularly subsection 6.3.3) considers ‘what-if’ scenarios that also address the possibility of the direct disposal of non-irradiated fuel.

It is unlikely that large amounts of un-irradiated or low burn-up fuel will require disposal. However, waste packages that include such fuel would exhibit higher reactivities than the irradiated fuel assumed in the Likelihood of Criticality project. Such waste packages may not be demonstrably sub-critical under conditions in which they are flooded with water. The use of multiple water barriers and/or neutron poisons in SF transport and storage containers may be sufficient to ensure that such fuel remains sub-critical during transport and disposal operations. However, fresh or low burn-up fuel may present a potential criticality concern for long periods after disposal (in excess of 10^6 years) and it may not be possible to take credit for the presence of multiple water barriers and neutron poisons over such periods. The sensitivity of the results of the Likelihood of Criticality project calculations to SF burn-up could be evaluated in the future to determine what controls will need to be placed on SF waste packages to ensure that post-closure criticality is unlikely. These controls may be in the form of minimum fuel burn-up requirements or limits on the amount of fuel placed in a disposal package.

Further options for the design and production of spent fuel disposal concepts suitable for exotics and metallic fuels within the UK inventory, together with the associated criticality safety controls, will shortly be considered as part of an ongoing project focused on disposal concept development (see [10] tasks 70 and 75 (exotics) and tasks 71 and 76 (metallic fuels)).

In summary, a range of administrative controls and design measures could be adopted as part of a demonstration of criticality safety during SF transport and disposal operations. Such controls include burn-up credit and associated confirmation requirements, the inclusion of neutron absorbing materials along with neutron flux traps, void fillers to limit water ingress, and multiple water barriers. Such options are being considered by RWM in research on SF management and further details are available in our Science and Technology Plan [10].

3.6 HEU and plutonium package fissile material limits

Although the UK Government has not yet decided whether or not to directly dispose of plutonium and HEU, we have undertaken research studies that give us confidence that these materials can be safely disposed of in the GDF.

In this section we discuss the proposed wasteform and packaging for separated HEU and plutonium.

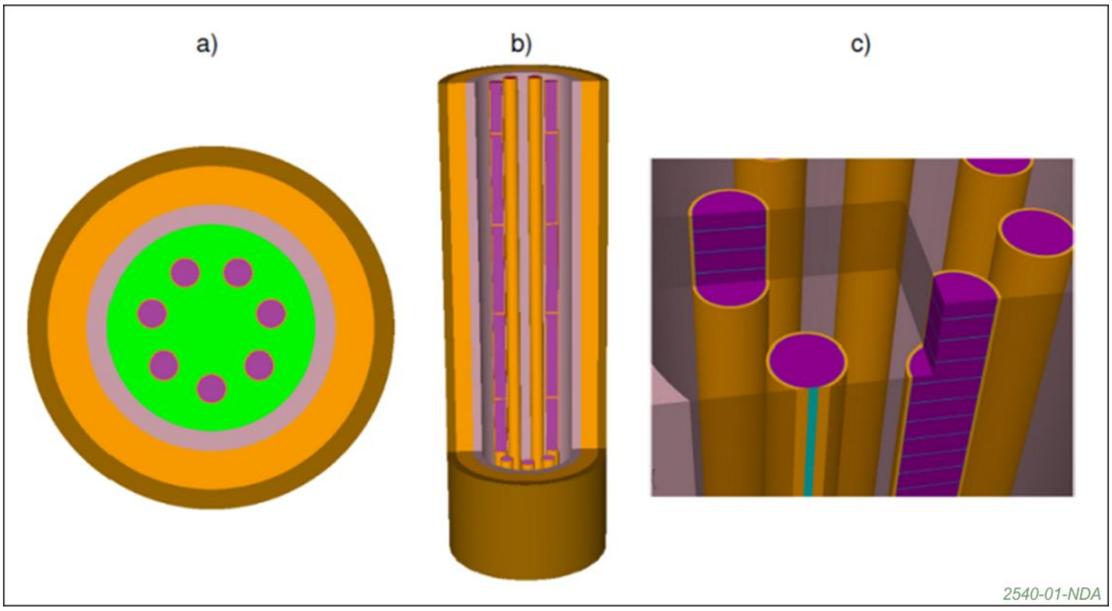
3.6.1 Packaging and wasteform assumptions

For planning purposes we have assumed plutonium and HEU will be processed into a ceramic wasteform and emplaced in a disposal container.

The development of disposal packaging concepts for HEU and plutonium wastes is still at an early stage, however, our approach has been to conduct sufficient research to underpin future governmental policy decisions on disposition of the UK's separated plutonium stocks. For the preparation of the plutonium/HEU Derived Inventory [39] it was assumed that a nominal 10 wt% of plutonium (~50 g) would be immobilised in a titanate-based ceramic to form a puck. The ceramic is assumed to include the neutron absorbers hafnium and gadolinium, as well as depleted uranium. Twenty pucks would be loaded into stainless steel cans and multiple cans of pucks (up to 28) would be encapsulated in glass within a larger 5 cm thick steel canister (the can-in-canister approach). These canisters would then be loaded into disposal containers of a similar design as for HLW and SF (copper or carbon steel containers depending on the host geology). The same wasteform and packaging concept is also assumed for HEU. The can-in-canister approach to the packaging pucks of plutonium and HEU is illustrated in Figure 8.

Figure 8(a) shows a slice through the package showing the outer copper container (brown), iron insert (orange), and inner stainless steel container (pink) with an arrangement of seven cans (purple) surrounded by borosilicate glass (green). Figure 8(b) shows a cut-away of the package and the different layers of cans, whilst Figure 8(c) shows the ceramic pucks (purple) within the inner cans (orange). In Figure 8(b) and (c) the borosilicate glass is not shown.

Figure 8 Conceptual illustration of the can-in-canister packaging concept for plutonium and HEU disposal, assuming a copper disposal container



Further options for the design and production of plutonium and HEU disposal concepts, and the associated criticality safety controls, are currently being considered as part of the ongoing project focused on concept selection (see [10] tasks 101 to 104).

3.6.2 Criticality safety research for plutonium and HEU disposal

Post-closure criticality safety can be demonstrated for the direct disposal of separated nuclear materials such as plutonium and HEU when they are processed into robust ceramic wasteforms.

As the current packaging concept assumes the plutonium and HEU will be packaged in a HLW/SF disposal container, the same criticality controls as discussed above may be used (such as multiple water barriers). However, for the current concept, the contributions to criticality safety would be provided by the stable, sub-critical wasteform and a long-lived container.

Packaging concepts for HEU and plutonium wastes are at an early stage of development, but it can be expected that variations in the fissile material content of waste packages will be carefully controlled and understood for any chosen concept. In the currently assumed form the mass and concentration of fissile material in the separated HEU and plutonium are likely to be much higher than that found in LHGW. On the other hand, the physical and chemical form will be well-defined, making measurement and control of fissile content more reliable, hence reducing the likelihood of over-batching errors[12]. A ceramic matrix would also provide a highly stable and robust (low leach rate and low moderator entry rate) material, highly resistant to any unfavourable changes due to events such as impact, fire, explosion or flooding.

As the current packaging concept assumes the HEU and plutonium would be packaged in the copper or carbon steel disposal containers, which are assumed to be transported in the DCTC; the same considerations as discussed in subsection 3.5.2 apply. If necessary, multiple water barrier arguments could be applied to the transport phase for HEU and plutonium wastes. However, the numerous barriers in the proposed wasteform, and its stable ceramic nature with embedded poisons, are expected to ensure sub-criticality any credible transport and GDF operations scenarios. Our research in this area (see [10], tasks 102 and 104) will be informed by similar studies that have been made in other countries, for example [65].

As discussed in detail later in subsection 6.3.4, work that assumed the can-in-canister packaging concept demonstrated how robust ceramic wasteforms are under GDF relevant conditions. In broad terms, if wasteform integrity is maintained, insufficient moderator can access the fissile material and subcritical conditions are ensured, even if we pessimistically assume that any beneficial neutron absorbing materials (the poisons) that may be required for transport and operational purposes are leached away over extended post-closure timescales.

4 Scenarios for Post-closure Criticality Safety Assessment

In this section we:

- note our historical studies of the likelihood and consequences of post-closure criticality (the results of our more recent research studies are presented separately in the subsequent two sections)
- describe both common features and specific aspects of our approach to using scenarios to assess post-closure criticality safety.

One of a variety of definitions of scenario is *'an outline or model of an expected or supposed sequence of events'* [66]. Criticality scenarios have been the focus of our work to support the derivation of fissile material limits on waste packages and to understand the likelihood and potential consequences of criticality after GDF closure. To this end, two broad types of scenario have been considered in our criticality safety studies:

- scenarios in which a sequence of events is assumed to result in redistribution of fissile material into a particular geometry. Those geometrical arrangements may be assessed in order to derive a minimum critical mass of fissile material. If assessed deterministically, using bounding pessimistic assumptions on moderation, reflection and interaction, and with the application of a suitable safety margin, a package limit can be set to avoid criticality, as described in subsection 3.3. Assessments undertaken probabilistically, supported by a more informed evaluation of system uncertainties, allow investigation of whether post-closure criticality has a low probability of occurrence, as described in Section 5 and applied in subsection 3.4.3.
- 'what-if' scenarios, in which a sequence of events is assumed to result in redistribution and accumulation of a super-critical mass of fissile material (however unlikely). These are defined in order to assess the consequences of criticality, as described in Section 6.

Subsection 4.1 gives the background and history of our research programme for hypothetical post-closure criticality scenarios. In subsection 4.2, the overall objectives for our development of post-closure criticality scenarios are discussed. Subsection 4.3 discusses the types of accumulations of fissile material necessary for a criticality. Subsection 4.4 provides some context about the timescales on which the GDF might be expected to evolve. Our approach to identifying criticality features, events and processes (FEPs) and constructing post-closure criticality scenarios is set out in subsection 4.5. Subsections 4.6 and 4.7 describe the criticality scenarios that we have considered in our assessments of the likelihood of criticality after GDF closure for disposal of LLW, ILW and DNLEU and SF, HLW, HEU and plutonium, respectively. Disposal facilities in higher strength rock, lower strength sedimentary rock and evaporite are discussed. Subsection 4.8 discusses the 'what-if' scenarios that have been considered in our work to understand the potential consequences of a hypothetical criticality in a GDF, again for a range of wastes and illustrative disposal concepts. Finally, subsection 4.9 introduces the Oklo natural reactors as an illustration of a scenario that resulted in natural critical systems approximately two billion years ago, which we can use to build confidence in our understanding of models.

4.1 Background to RWM's work on post-closure criticality

RWM (and its predecessor organisations) has worked since the early 1990s on developing a capability to understand and to be able to demonstrate the post-closure criticality safety of the GDF.

Initial studies on post-closure criticality were conducted in the 1990s and considered ILW in a higher strength rock environment. The studies are summarised in a topical report [67], supported by 19 detailed reports. The aim of the work was to develop the understanding, data, models and methods necessary to assess the post-closure criticality safety of the GDF for ILW and certain LLW. The scope of work included assessment of mechanisms, involving relocation and accumulation processes, which have been identified as having the potential to lead to a criticality, and work on the possible effects of a criticality, should one occur, and its impact on GDF performance. The studies concluded that the potential for a criticality would be low and that, even if a criticality did occur, its impact on GDF performance would not be significant. However, the work on consequences was not comprehensive.

From 2001, the research focus was on modelling the consequences of post-closure criticality, from ILW in a higher strength rock environment. However, by 2010, some work was underway on assessing the likelihood of criticality in illustrative environments, although still limited to ILW; this was subsequently reported [68, 69]. The research programme was termed Understanding Criticality under Repository Conditions (UCuRC), and is discussed further in subsection 6.1. The aim was to obtain a better understanding of the processes that would control the nature and magnitude of a criticality under the particular conditions arising post-closure in the GDF containing ILW.

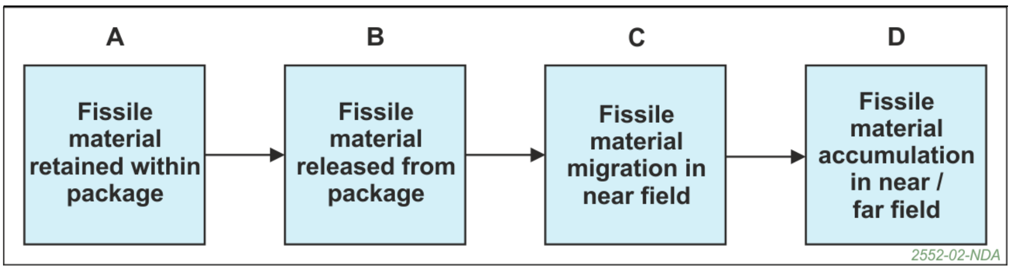
In 2010, it was recognised that further research was required on both likelihood and consequences, covering all higher activity materials and all three illustrative concepts. Two independent, but aligned, research projects were initiated in 2011: one assessing the likelihood of criticality (described in section 5); the other covering further modelling of the consequences of a hypothetical criticality (described in subsection 6.3). The understanding gained has since been applied in a safety assessment, see subsection 7.1. The conclusion drawn from the totality of this work was that, for all higher activity wastes disposed of in the three illustrative host rocks, post-closure criticality would be a low likelihood and a low-consequence event.

4.2 Objectives for scenario development

For post-closure criticality to occur, substantial degradation of waste packages and/or relocation of fissile or wasteform materials would be required. Various 'what-if' scenarios for this have been considered.

The stages in which critical accumulations of fissile material may occur are summarised in Figure 9, which is based on the expected evolution of packages and the GDF.

Figure 9 Stages in which critical accumulations of fissile material may occur



These various stages have been considered in our criticality safety studies:

- Stages A and B have been assessed deterministically to determine maximum safe accumulations in ILW packages (section 3).
- Stages A, B and C (and to a lesser extent Stage D) have been assessed probabilistically to investigate the likelihood of critical accumulations arising during the expected evolution of the GDF (subsection 3.4.3 and section 5).
- Stage D has been the main focus in using 'what-if' scenarios to assess the consequences of accumulations of critical masses of fissile material (Section 6). Such scenarios can also be used to consider the consequences of hypothetical accumulations whose likelihood cannot currently be assessed because the sequence of events is uncertain or unexpected; examples would be as a result of human intrusion or as a result of precipitation at 'chemical fronts' (as at Oklo, see subsection 4.9). Stages A and B have also been assessed using 'what-if' scenarios, specifically for SF in-package criticality and ILW stack slumping respectively.

4.3 Accumulations required for criticality

A critical system requires sufficient fissile material, sufficient moderator and a lack of neutron absorbers. For ILW and HLW there is a large safety margin to reaching a critical system in the post-closure GDF, even allowing for any long-term degradation of waste and migration of fissile material.

The parameters (concentration, mass and geometry) for a critical system depend strongly on composition. They also depend on the arrangement of the materials. In general, a critical system requires:

- sufficient fissile material
- sufficient moderator
- a lack of neutron absorbers
- sufficient physical size to reduce the effect of neutron leakage (so that enough neutrons generated by fission are available within the fissile region to lead to further fission).

The various stages noted in subsection 4.2 can be assessed to determine what combination of materials could give rise to a critical accumulation. We then use well-established, internationally recognised and validated, techniques (developed over about 40 years for reactor physics and criticality assessments) to calculate the combination of parameters required to achieve a criticality.

It is also possible to compare calculations using different computer code systems [31, 45] to ensure that there is high confidence in the predictions. The individual codes have been benchmarked using an international database of criticality experiments.

This understanding can be used to inform us as to what specific conditions need to be avoided in order to ensure criticality safety.

The combination of conditions required for criticality is hard to attain, suggesting that achieving a critical system, when the initial packaged state is not critical, is unlikely. However, a critical system has occurred in nature (see subsection 4.9), although this was long ago (about two billion years) when the natural ^{235}U 'enrichment' level was far greater[19] than it is today.

For modelling the accumulation of fissile materials, data on minimum critical masses and concentrations in different components of the GDF (waste packages, engineered barriers and host rock) have been obtained using neutron transport codes, and from criticality reference books. These data include information on minimum critical masses and concentrations, which can be used to judge whether critical systems could develop for the range of post-closure criticality scenarios under consideration. Given the large uncertainties in the geometry of potential fissile material accumulations, we have adopted a cautious approach in that simple optimally moderated and reflected spherical, cylindrical or slab configurations have been assumed for the majority of the analyses. For 'what-if' in-package scenarios, some more complicated geometrical configurations have also been considered, specific to SF, plutonium and HEU wastes.

The main fissile radionuclides to consider in the disposal system assessment are ^{239}Pu and ^{235}U, which make up the major part of the fissile inventory. For the disposal system application, the groundwater acts as a moderator (but also as an absorber of neutrons). Another significant neutron absorber in the disposal system is ^{238}U, which forms 99.28 wt% of natural uranium. Uranium in water is always sub-critical unless the ^{235}U has been enriched above its natural fraction (0.71 wt%).

Figure 10 shows the results of calculations [70] to obtain the parameters for just-critical configurations (at a $K_{effective}$ of 1) of ^{239}Pu (the red curve; other systems are also shown) which it is assumed has accumulated in a cylinder in saturated backfill[20], without any other neutron absorbing materials (such as ^{238}U, steel) present. The plutonium (and the uranium in other systems) is in the form of dioxide. At masses below the curves shown in Figure 10, and concentrations to the left (lower concentrations), systems/accumulations would be sub-critical (a $k_{effective}$ of less than 1). At accumulations above and to the right of the curves shown, systems could be critical (have a $K_{effective}$ of above 1). The figure shows that there are limits on both mass (the minimum critical mass) and the concentration[21], which must be exceeded before a criticality is possible. While the minimum critical mass is relatively small (at ~1 kg), the minimum concentration for a criticality in a cylindrical system is quite high (~10 kg/m^3), much higher than the likely concentration of ^{239}Pu in ILW. Taking account of neutron absorbers will cause both the critical mass and the minimum concentration to increase. Above specific neutron absorbing material concentrations, a criticality is no longer possible irrespective of the size and mass of the system.

Figure 10 shows that the results for ^{239}Pu are close to bounding for any fissile inventory. Calculations for the accumulation of ^{235}U show the effect of the neutron absorber ^{238}U. The minimum critical mass of ^{235}U increases by about a factor of five going from pure ^{235}U to an isotopic composition typical of fresh AGR or PWR nuclear fuel (3% ^{235}U, 97% ^{238}U)[22] as denoted by the green line; the required mass of uranium increases by about a factor of 150.

The evaluations for accumulation in backfill assume a high porosity, which can be filled with either water or the accumulating material. Rock masses have lower porosity, so if an

19 Owing to the time they occurred, roughly 2 billion years ago, the Oklo natural reactors are estimated to have contained natural uranium with an enrichment of around 3.6% ^{235}U, which is close to the enrichment of modern nuclear reactor fuel.

20 The backfill assumed in the calculations is NRVB, the Nirex Reference Vault Backfill, a cementitious material developed by Nirex (which became NDA RWMD in 2007 and RWM in 2014).

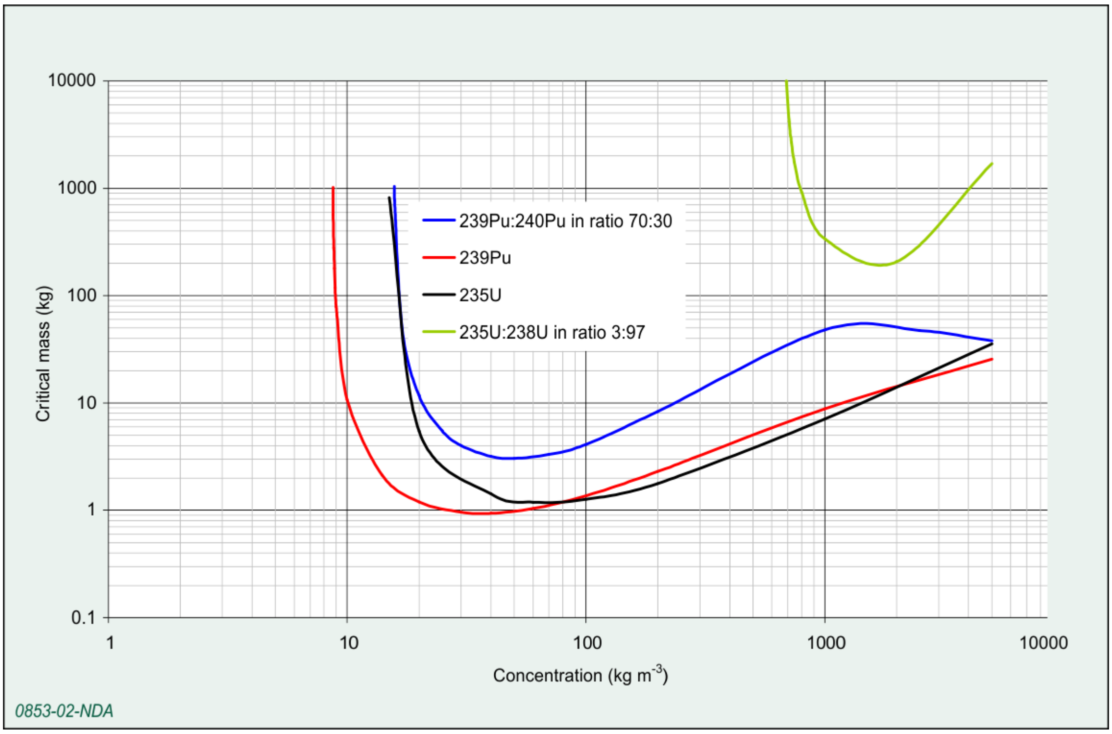
21 The minimum concentrations for criticality in saturated NRVB are slightly higher than the values in pure water, which are 7 kg/m^3 for ^{239}Pu and 11 kg/m^3 for ^{235}U.

22 This factor is derived for a homogeneous distribution of fissile material in the backfill; it is lower in some other geometries.

accumulation were to occur in the host rock (for example, through deposition in small cracks) significantly higher minimum critical masses are required.

The total estimated fissile content of the ILW is estimated to be 13.5 tonnes, dispersed through ~470,000 m^3 of waste and packaging (Table 1). The fissile material will be well spread throughout the volume. Thus, the average concentration of fissile material in the ILW will be less than 0.03 kg/m^3, which is more than 300 times below that necessary to sustain a criticality under optimum conditions in, for example saturated NRVB. Even for plutonium contaminated material, the average concentration would be a factor of more than 50 below that necessary to sustain a criticality in optimum conditions (for example see Figure 10). Given that the maximum loading of fissile material in individual ILW packages will be such as to prevent a criticality while the original geometry is maintained, there is a large margin (in terms of both mass and concentration) to reaching a critical state in the post-closure period, even allowing for any long-term movement of the fissile materials.

Figure 10 Critical masses of plutonium and uranium for cylindrical fissile systems in saturated NRVB (fissile material in oxide form). Figure produced from data presented in [70]



Similar considerations apply to HLW, which has an average fissile concentration in the wasteform of ~0.01 kg/m^3, broadly comparable to ILW. In the case of HLW the fissile material is also intimately mixed and immobilised with neutron absorbers (boron in the glass and some of the fission products) in a high integrity package.

4.4 Timescales for evolution of the geology and hydrogeology

At the depth of the GDF, the geosphere is expected to be relatively stable, so broad observations can be made about the likely stability over timescales relevant to the post-closure phase of the GDF.

GDF post-closure criticality scenarios depend on the evolution of conditions in the near field of the GDF and the migration of fissile radionuclides over long time periods. The choice of timescales over which to undertake criticality scenario assessment calculations is not straightforward. For instance, mobilisation and dispersion of radionuclides could occur on timescales from tens of years up to billions of years, depending on the type of waste package and GDF conditions. Also, uncertainties in GDF evolution tend to increase with time and the reliability of calculations over very long timescales can be questionable.

For example, the long-term performance of the GDF will depend on the stability of the geosphere. Natural processes such as tectonics, uplift or subsidence and erosion, and climate change, particularly future glaciations, may affect the geosphere in a UK geological environment over the next million years [4]. In the absence of a disposal site, the effects of such processes on geosphere and barrier system performance are difficult to predict. However, at depths under consideration for the GDF, the geosphere is less dynamic than shallow geological or surface environments and natural processes will occur slowly. The following broad observations can be made about the likely stability of the geological environment of the GDF [4]:

- the UK is situated in a tectonically quiet region and is expected to remain so for many millions of years
- the next period of volcanic activity in the UK is not expected to occur for at least some millions of years
- the GDF will be constructed such that waste will not be emplaced in the vicinity of larger fractures, identified during site characterisation, which are more likely to be affected by future seismic activity
- the extent of any uplift and erosion before the next glaciation for an appropriately sited GDF, and over the next million years, will be substantially less than the depth of the GDF
- estimates of the extent of erosion caused by glaciation, which is not expected in the UK for 200,000 years or more, are significantly less than the design depth of the GDF, although glacial loading and unloading could affect fracture properties and groundwater flow in the geosphere.

The extent and timing of such changes and their potential impacts on GDF performance are uncertain, especially in the absence of a disposal site. However, it is clear that, for a carefully selected site, the contribution to criticality safety from the geosphere in the long term could be achieved.

It is recognised that future safety assessments may not include detailed quantitative analysis beyond a few hundred thousand years because of increases in uncertainty associated with the potential effects of climate change. Indeed, future safety assessments may rely on qualitative and simple quantitative arguments about the likelihood and consequence of criticality in the GDF in the very long term in combination with probabilistic modelling on timescales of a few hundred thousand years.

In our criticality research, some calculations of the likelihood of a criticality (see Section 5) have been run out to 100 million years, primarily to scope the effect of failure of high integrity copper containers for SF by corrosion - which may take a very long time. However, it should be noted that there can be little confidence in the results of calculations this far into the future. Whilst detailed calculations are presented, it should be understood that results beyond a few hundred thousand years, or after there has been a significant change in the hydrological boundary conditions (such as is possible during an extensive glacial period), should only be regarded as indicative of long-term performance. Our eventual site-specific environmental safety case, currently in a generic form [71], may use such information to inform a qualitative discussion on the expected continued evolution of the disposal system. Throughout this status report all assessment plots that extend beyond 200,000 years have been appropriately labelled to indicate this important timeframe consideration.

4.5 Approach to criticality FEP and scenario identification

In order to understand the likelihood and consequences of post-closure criticality we require a range of post-closure criticality scenarios to assess against. These have been derived through a FEP analysis approach.

The combinations of events and processes that would need to occur for neutron reactivity to increase after GDF closure are similar for each type of waste package, disposal concept and geological environment that we are considering. Generally, groundwater would need to enter the waste packages after GDF closure in order to initiate the wasteform dissolution and degradation processes that would be required for substantial changes in reactivity to occur. Unless the waste container design includes openings (such as for ventilation, as in all ILW packages) waste container failure (likely through corrosion) would be required to allow water ingress. Degradation of the wasteform following water ingress could result in relocation of fissile and other materials within the disposal package, which could lead to changes in package reactivity. Also, fissile material may be released from waste packages. If the fissile material is dispersed, reactivity would decrease. However, fissile material (potentially from more than one waste package) may accumulate at specific locations within the EBS or the geosphere, resulting in increased reactivity. If sufficient fissile material is involved in such accumulations, critical systems may develop. On the basis of this understanding, we have defined FEPs for LLW, ILW and DNLEU and SF, HLW, HEU and plutonium disposal concepts in each geological environment in terms of the following groups:

- FEPs that could result in water entry into a waste package (for example, the presence of ventilation openings or the occurrence of package failure mechanisms)
- FEPs that could result in changes in reactivity following water entry into the waste package (such as degradation leading to the relocation of fissile material, neutron absorbers, neutron reflectors and / or neutron moderators)
- FEPs that could result in the migration and accumulation of fissile material outside a single waste package (for example, accumulation by precipitation, sorption, filtration or gravitational settling)
- FEPs that could result in the migration and accumulation of fissile material from more than one waste package.

Each of these criticality FEP groups has been considered in terms of mechanical, chemical, thermal, gas-related, hydrological, radiological and microbiological events and processes that might occur for the different types of waste package, disposal concepts and geological environments. Detailed descriptions of these FEPs are presented in the reports on the likelihood of criticality following LLW, ILW and DNLEU disposal [72] and SF, HLW, HEU and plutonium disposal [73].

Post-closure criticality scenarios have been constructed based on judgments about the importance of each of these FEPs. It is recognised that a comprehensive FEP analysis would include consideration of FEPs external to the GDF that could alter conditions in the disposal facility and affect the potential for criticality. However, the effects and likelihood of such external FEPs are considered to be specific to the GDF’s location. For example, the effects of climate change, the frequency and magnitude of seismic events and the likelihood and impacts of human intrusion are site-specific. Thus, although such factors have been identified in the FEP analysis, they are not currently included in the scenario assessment conducted in the current generic phase of the work programme because of the large uncertainties associated with their likelihood and effects. Such factors will be considered in the scenarios assessment approach when site-specific data are available.

Based on the FEP analysis, three broad post-closure criticality scenarios have been defined in each geological environment, these are:

- increased reactivity inside a single waste package
- accumulation of fissile material outside a waste package
- accumulation of fissile material from multiple waste packages.

GDF evolution and descriptions of post-closure criticality scenarios relating to LLW, ILW and DNLEU and SF, HLW, HEU and plutonium disposal are presented in subsections 4.6 and 4.7, respectively.

4.6 Post-closure criticality scenarios for LLW, ILW and DNLEU disposal

To determine whether critical systems could develop through the range of post-closure scenarios considered we have applied a range of approaches, from high-level judgements about scenario credibility to probabilistic modelling.

This section provides high-level descriptions of the evolution of conditions in the GDF for LLW, ILW and DNLEU disposal (the low heat generating module of the GDF).

Key events and processes relating to how conditions are expected to change in disposal facilities in higher strength rock, lower strength rock and evaporite are discussed in turn below and in more detail in [72].

4.6.1 LLW, ILW and DNLEU disposal in higher strength rock

For LLW, ILW and DNLEU disposal in higher strength rock post-closure scenarios considered are: increased reactivity inside a waste package, accumulation of fissile material outside a waste package, and accumulation of fissile material from multiple waste packages.

The illustrative concept for LLW, ILW and DNLEU disposal in higher strength rock involves stacking the waste packages in vaults and backfilling the vaults using NRVB, a cement-based material. After backfilling, the disposal area will start to resaturate; groundwater flow into the disposal area will be predominantly through fractures in the rock. The incoming groundwater will rapidly equilibrate with the NRVB, resulting in the development of alkaline conditions. Reducing conditions will soon be established as a result of, for example, oxygen consumption by corrosion reactions.

Once the vaults have resaturated, alkaline and reducing conditions will limit radionuclide solubility. Only small concentrations of uranium and plutonium would begin to be released into the backfill via diffusion through vents in the containers. Waste packages will gradually corrode under disposal conditions and will eventually fail such that flow could become established through the wasteform, resulting in the advection of mobile materials.

Settling of solid plutonium and uranium through waste packages could occur if voids form as grout is dissolved and removed from waste packages (referred to as a slumping scenario). One way of assessing the validity of this slumping scenario is to examine available qualitative and quantitative evidence for the formation of dissolution cavities and void spaces, such as caves, in natural systems. Voids and caves are particularly abundant features in areas of limestone karst. Therefore a review was undertaken of observations and modelling of the rates of void formation in limestone karst regions[23] (see Appendix F of [72]). This review indicated that the rate of water flow is the primary control on void and cave formation. The formation of large dissolution caves involving the removal of significant volumes of solid material requires the flow of chemically aggressive water to be sufficiently high that chemical equilibrium between the waters and the rocks is not achieved and mineral dissolution rates remain high. If water flow is absent, or if flow rates are low, chemical equilibrium will be approached and dissolution rates will fall substantially. Groundwater flow rates in limestone karst areas are much higher (by several orders of magnitude) than those envisaged in higher-strength or lower-strength host rocks deemed to be appropriate for the geological disposal of radioactive wastes. Even if a fracture in a higher-strength host rock was to focus water flow through a single waste package, or through a stack of waste packages, flow and dissolution rates would still be low by comparison with karst areas. The overall conclusion is that the formation of significant voids would not occur in an appropriately sited GDF. If it occurred at all, the removal of sufficient material to cause slumping would take well in excess of one million years.

Strong sorption to corrosion products, waste encapsulation material and backfill will slow the migration of dissolved uranium and plutonium through the engineered barrier system, however organic complexing agents derived from the degradation of cellulosic materials in wastes may increase radionuclide mobility. Naturally-occurring colloidal organic materials dissolved in groundwater may also affect radionuclide mobility. These complexing effects are discussed in the Radionuclide Behaviour Status Report [5].

Cracks in the backfill will tend to channel groundwater flow, and plutonium and uranium would be advected in the direction of the flow in the cracks, with advection at lower rates in the rock matrix. Dissolved uranium and plutonium will eventually be released to the host rock, where migration will be retarded by sorption, precipitation and diffusion into the rock matrix.

Based on consideration of these GDF evolution processes, scenarios involving increased reactivity inside a waste package, accumulation of fissile material outside a waste package and accumulation of fissile material from multiple waste packages can be constructed. The key stages in the development of these scenarios are illustrated in the event tree shown in Figure 11. The grey boxes indicate criticality scenarios involving fissile material from a single package and the green boxes indicate scenarios involving fissile material from multiple packages.

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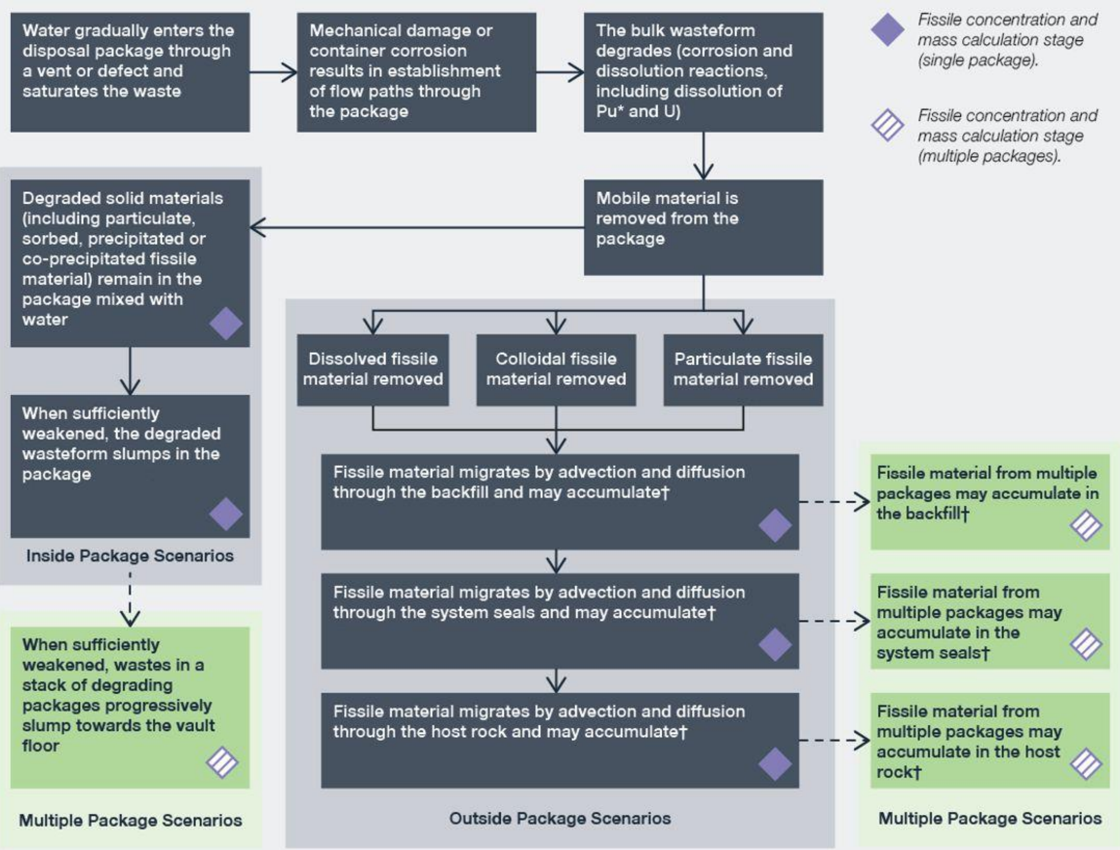
23 Karst regions are a type of landscape/geological environment that exhibits characteristics such as voids (caves and caverns) caused by chemical dissolution of the rock. Karsts form in soluble rocks with a permeability structure dominated by conduits dissolved from the rock and organised to facilitate the circulation of fluids. It is emphasised that karst areas themselves are not considered suitable for the GDF. The conduct of the above mentioned review does not imply any intention to dispose of radioactive wastes in areas of limestone karst.

Figure 11 Event tree showing fissile material redistribution and accumulation scenarios for LLW, ILW and DNLEU disposal in higher strength rock



* Radioactive decay of ^{239}Pu to ^{235}U may be significant for all scenarios
† Accumulation may occur as a result of sorption, precipitation, filtration or settling, according to the material properties and geochemical and hydrogeological conditions.

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4.6.2 LLW, ILW and DNLEU disposal in lower strength sedimentary rock

The same scenarios apply for LLW, ILW and DNLEU disposal in lower strength sedimentary rock, except that mass transfer will in general be by diffusion, rather than advection.

The concept for LLW, ILW and DNLEU disposal in lower strength sedimentary rock involves stacking the waste packages in vaults and backfilling the vaults using a cementitious grout. The waste package stack height would be lower than in vaults in higher strength rocks because excavations would be smaller. Unlike in higher strength rock, transport is expected to be dominated by diffusion rather than advection. After backfilling, the disposal vaults will start to resaturate, but the rate of resaturation will be low because of the low permeability of the host rock. Oxygen in the vaults will be consumed by corrosion and other processes, such as microbial activity. Alkaline conditions will develop as the incoming groundwater reacts with the cementitious backfill.

The containers will gradually corrode and lose their integrity. As a result, mobile radionuclides will be released from the waste packages in groundwater and will start to migrate through the engineered barrier system and into the host rock. Scenarios involving increased reactivity inside a waste package, accumulation of fissile material outside a waste package and accumulation of fissile material from multiple waste packages are similar to those shown in Figure 11 for the higher strength rock example, except that mass transfer is by diffusion only and rock creep may affect package integrity.

4.6.3 LLW, ILW and DNLEU disposal in evaporite

For LLW, ILW and DNLEU disposal in evaporite, compaction of waste packages is considered. However, relocation of fissile and other materials to form a critical configuration outside a waste package cannot be envisaged in a dry GDF.

The concept for LLW, ILW and DNLEU disposal in evaporite also involves stacking the waste packages in vaults, although stack heights would be lower than in vaults in lower strength sedimentary rocks. It is assumed that no backfilling will be required within the disposal vaults, because natural rock creep will close the excavations over time.

In an undisturbed evaporite, groundwater transport occurs only through the rock matrix (since fractures are largely absent, unless significant bedding is present) and flow rates are typically extremely low or even non-existent. Groundwater may be present, typically as brines in discrete pockets, and those systems may be saturated. However, the groundwater or brine is likely to be held within isolated locations, so there will be little mobile water in any one location. In the absence of connected porosity in an undisturbed evaporite, there will be no pathways for radionuclide migration. In the early post-closure phase, dry engineered barrier system evolution will be ensured by shaft and access-tunnel seals that prevent water entry from overlying formations and waste package corrosion will be limited.

Rock creep will reduce voids, sealing the openings around and within the GDF. This self-sealing behaviour means that any pathways that might enable more rapid migration of fluid, and hence radionuclide transport, away from the engineered barrier system are typically short-lived. Evaporite host rocks are able to provide a high degree of containment over the very long term.

Multiple breached waste packages are expected due to compaction and as a result of various chemical degradation processes. However, by the time significant waste package degradation or breach has occurred, complete containment of the waste in the GDF will be provided by the host rock.

The absence of accessible groundwater greatly influences the types of post-closure criticality scenario that could develop. Weakening of a degrading waste package, combined with pressure applied by rock creep, could result in compaction of remaining solid materials, which could affect reactivity. However, if there is no appreciable water present then radionuclides will not move far from a failed waste package. Relocation of fissile and other materials to form a critical configuration outside a waste package cannot be envisaged in a dry GDF.

4.7 Post-closure criticality scenarios for SF, HLW, HEU and plutonium disposal

To determine whether critical systems could develop through the range of post-closure scenarios considered we have applied a range of approaches, from high-level judgements about scenario credibility to probabilistic modelling.

This section provides high level descriptions of the evolution of conditions in the GDF for SF, HLW, HEU and plutonium.

Key events and processes relating to how conditions are expected to change in disposal facilities in higher strength rock, lower strength rock and evaporite are discussed in turn below and in more detail in [73].

4.7.1 SF, HLW, HEU and plutonium disposal in higher strength rock

For SF, HLW, HEU and plutonium disposal in higher strength rock, post-closure scenarios considered are: increased reactivity inside a waste package, accumulation of fissile material outside a waste package, and accumulation of fissile material from multiple waste packages.

The illustrative disposal concept for SF, HLW, HEU and plutonium disposal in higher strength rock involves vertical emplacement of individual copper disposal containers (Variant 1) in deposition holes drilled from tunnels, with each disposal container surrounded by bentonite. The disposal tunnels will be backfilled with a mixture of crushed rock and bentonite.

After emplacement, the bentonite buffer and tunnel backfill will begin to resaturate, causing the bentonite to swell. A swelling pressure will develop as the buffer expands to seal the disposal container in the deposition hole. On saturation, the buffer will provide a low-permeability barrier around the container. Hydraulic conditions in the near field will slowly equilibrate with those in the surrounding host rock after saturation of the buffer and backfill.

If fluid flow through fractures intersecting deposition holes is sufficiently large, then the bentonite may be susceptible to piping and erosion. These processes have the potential to remove significant amounts of bentonite from a deposition hole and, hence, reduce the ability of the buffer to protect the container. As far as possible, the intersection of features of such high hydraulic conductivity will be avoided, see the Engineered Barrier System status report [3]. Such features are often referred to as layout defining features. If a deposition hole does intersect such a feature the deposition hole will not be used.

Chemical reactions between groundwater and bentonite minerals are expected to result in chemical buffering of the bentonite pore water to a near-neutral or slightly alkaline pH. In the long term, the capacity for chemical buffering of the bentonite by reaction with groundwater will diminish as the reactants in the bentonite are exhausted and, depending on the chemical composition of the groundwaters, the composition of the buffer might be altered. Such alterations could affect the swelling pressure and hydraulic conductivity of the buffer.

Oxygen will be exhausted quickly as a result of redox reactions with dissolved reducing species and mineral impurities in the bentonite, and as a result of aerobic corrosion of the copper disposal container. Reducing conditions will be maintained by the ingress of reducing groundwater. Development of a reducing redox potential in the vicinity of the disposal container will substantially slow the corrosion rate of copper, leading to long container lifetimes. Aggressive species, such as sulphides generated by microbial activity, could accelerate corrosion, but the transport of these species to disposal container surfaces will be limited by the low permeability of the bentonite. Generally, the copper containers are expected to maintain their integrity and provide full radionuclide containment for at least 100,000 years, if not significantly longer.

Seismic events caused by earthquakes or glacial loading and unloading could contribute to container failure as a result of shear along fractures that intersect container deposition holes (see the Geosphere Status Report for further discussion [4]). However, the buffer fills the space between the container and the host rock, and is designed to protect the container and the wastes from the effects of deformation. Also, large faults and potentially significant fractures will, as far as possible, be avoided when locating deposition holes. In this way the potential for earthquakes to affect the disposal container will be minimised.

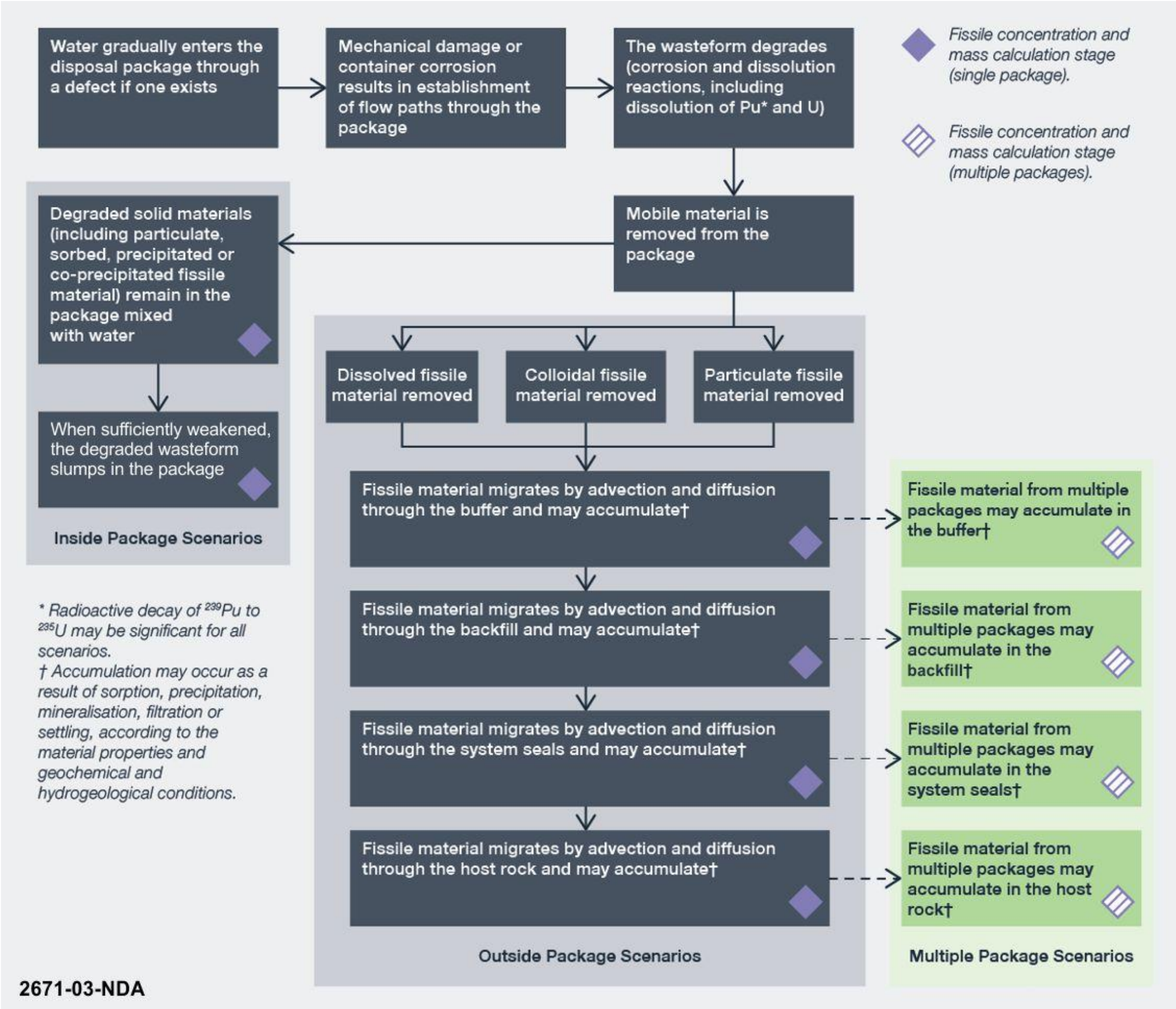
If a copper container were to fail, pore waters would come into contact with the cast iron insert present inside the container and would initiate dissolution of the wasteform. In general, the release rates of radionuclides such as uranium and plutonium will be restricted because of their low solubility under expected reducing conditions.

The transport of any uranium and plutonium released from the wasteform will be retarded by a combination of sorption on, and co-precipitation with, secondary phases formed by the degradation of waste package materials, as well as by sorption on surfaces provided by the bentonite buffer. Uranium and plutonium transport through the bentonite will occur primarily by diffusion, unless the bentonite has degraded, before eventual release into the host rock.

Degradation of bentonite could cause the formation of bentonite colloids. Colloids could also be generated by the corrosion of copper and steel in the waste packages. Such colloids might have a high sorptive affinity for uranium and plutonium. In addition, degradation of the HLW and SF matrices has the potential to produce uranium and plutonium colloids. Provided the bentonite swelling pressure is maintained, the buffer will filter out and immobilise any uranium and plutonium colloids generated within waste containers.

Based on consideration of these GDF evolution processes, scenarios involving increased reactivity inside a waste package, accumulation of fissile material outside a waste package and accumulation of fissile material from multiple waste packages can be constructed. The key stages in the development of these scenarios are illustrated in Figure 12. The grey boxes indicate criticality scenarios involving fissile material from a single package and the green boxes indicate scenarios involving fissile material from multiple packages.

Figure 12 Event tree showing fissile material redistribution and accumulation scenarios for SF, HLW, HEU and plutonium disposal in higher strength rock



4.7.2 SF, HLW, HEU and plutonium disposal in lower strength sedimentary rock

The same scenarios apply for SF, HLW, HEU and plutonium disposal in lower strength sedimentary rock, except that mass transfer will in general be by diffusion rather than advection.

The disposal concept for SF, HLW, HEU and plutonium disposal in lower strength sedimentary rock involves emplacement of carbon steel disposal containers in horizontal disposal tunnels. The disposal tunnels would be backfilled with bentonite pellets.

After emplacement, water will enter the disposal tunnels and deposition holes from the host rock and the bentonite buffer around the disposal containers will swell. The swelling will increase the buffer density and the mechanical strength, allowing the buffer to resist the pressure caused by creep of the surrounding host rock. The permeability of the saturated bentonite will be low, such that diffusion is the dominant solute transport mechanism. The pore waters will generally have a neutral or slightly alkaline pH provided by the buffering capacity of the bentonite and minerals in the host rock.

The carbon steel disposal containers will begin to corrode after emplacement. Initially, the corrosion rate will be relatively high under aerobic conditions, but the corrosion reaction will consume oxygen and the buffer pore waters will quickly become reducing. The corrosion of carbon steel occurs at a much slower rate under anaerobic conditions and the disposal packages are expected to provide complete radionuclide containment for in excess of 10,000 years, or at least 1,000 years under worst-case conditions.

Once the carbon steel waste packages have been breached pore waters will begin to leach radionuclides from the wasteforms. The release rates of uranium and plutonium will be restricted because of their low solubility under expected reducing conditions (see the Behaviour of Radionuclides and Non-radiological Species in the Groundwater Status Report [5] for further details). The transport of uranium and plutonium after release from the wasteform will be retarded by sorption on and co-precipitation with the products of steel corrosion and sorption on the clay minerals in the bentonite buffer. Migration of uranium and plutonium through the low-permeability bentonite and host rock will be diffusion-dominated.

Colloids could be generated by corrosion and degradation of the waste packages and wasteform, which could facilitate uranium and plutonium transport. However, the bentonite buffer is expected to filter colloids and prevent them from moving away from the site of their generation. Similarly, the host rock will act to filter colloids.

Scenarios involving increased reactivity inside a waste package, accumulation of fissile material outside a waste package and accumulation of fissile material from multiple waste packages are similar to those shown in Figure 12 for the higher strength rock, except that mass transfer would be by diffusion only.

4.7.3 SF, HLW, HEU and plutonium disposal in evaporite

For SF, HLW, HEU and plutonium disposal in evaporite compaction of waste packages is considered. Relocation of fissile and other materials to form a critical configuration outside a waste package cannot be envisaged in a dry GDF.

The disposal concept for SF, HLW, HEU and plutonium disposal in evaporite involves emplacement of carbon steel disposal containers (Variant 2) in horizontal disposal tunnels. The disposal tunnels would be backfilled with crushed rock.

Rock creep will begin immediately after excavation due to the presence of differential stress caused by the creation of void spaces. It is expected that creep and compaction will reduce the permeability of backfilled tunnels and seals to values similar to that of the host rock. Elevated temperatures generated by the SF and HLW will accelerate the creep rate and sealing of the GDF. SF, HLW, HEU and plutonium containers are expected to resist the mechanical effects of creep closure and maintain their integrity until processes such as corrosion have reduced their structural strength. The disposal containers are not expected to be significantly degraded until timescales conceivably exceeding a hundred thousand years after disposal.

As a consequence of their low permeability and porosity, the total amount of liquid in evaporite environments is very low. The absence of accessible groundwater greatly influences the types of post-closure criticality scenario that could develop. Weakening of a degrading waste package combined with pressure applied by rock creep could result in compaction of remaining solid materials, which could affect reactivity. However, if there is no appreciable water present then radionuclides would not move far from a failed waste package. Relocation of fissile and other materials to form a critical configuration outside a waste package cannot therefore be envisaged in a dry GDF.

4.8 'What-if' post-closure criticality scenarios

'What-if' scenarios provide understanding about the consequences of post-closure criticality events in the unlikely event that they should occur.

The use of 'what-if' scenarios is a requirement of the environment agencies' Guidance on Requirements for Authorisation [17].

The 'what-if' scenarios are based on the same underlying FEPs as the criticality scenarios discussed above in that they consider how evolution of the GDF could lead to criticality, but they do not form part of the formal analysis of the likelihood of criticality. We therefore define a 'what-if' scenario to be:

> *"a supposed (i.e. assumed) outcome of a sequence of events whereby, within a localised volume of the GDF or the surrounding host rock, a critical configuration of fissile materials is reached."*

The analysis of any such scenario does not imply that it will occur, in fact all of the scenarios are expected to be low likelihood. Also, the higher the accumulated mass assumed, the lower the likelihood. While the 'what-if' scenarios are not used to evaluate likelihood, they are closely aligned to the probabilistic assessments undertaken. This alignment has been a key component of our research programme in working towards the analysis of risk, as discussed in subsection 2.2 and Section 7.

As for the probabilistic assessments, our 'what-if' scenarios have been chosen to enable analysis of a range of different wastes and different illustrative disposal concepts. Three general 'what-if' scenarios have been considered:

- the accumulation scenario. It is assumed that fissile material is mobilised from one or more degraded waste packages and then transported in groundwater before accumulating in a localised region of the GDF or the surrounding host rock. This 'what-if' scenario can be postulated for any waste and any disposal concept that would saturate with groundwater.
- the stack-slumping scenario. It is assumed that, once the encapsulant material within a stack of waste packages is sufficiently degraded, the remaining fissile material slumps with gravity to the base of the stack. This 'what-if' scenario can only be postulated for waste packages that are emplaced in stacks (that is, LLW, ILW and DNLEU), and where a mechanism exists for significant degradation of the

structure of the stack (for example, dissolution of encapsulant or extensive corrosion of the steel containers).

- the in-package scenario. This assumes that some change occurs within a single package, whereby a critical configuration develops. This could include, for example, package flooding or the removal of neutron absorbers. This 'what-if' scenario can only be postulated for waste packages containing sufficient fissile material (above the minimum critical mass). It is mainly applicable to SF, plutonium or HEU packages, although it could also potentially apply to a small number of ILW or DNLEU (the LEU component) packages.

To understand the consequences of post-closure criticality from these 'what-if' scenarios we have used a staged approach:

- initially, we consider idealised realisations of the 'what-if' scenarios to understand the conditions that would have to develop for a critical configuration of fissile material to occur. Typically we achieve this utilising what we refer to as static criticality calculations which may include pessimisms, such as the assumption of a spherical geometry for the accumulation scenario or the presence of un-irradiated fuel for the in-package scenario for SF.
- where the analysis shows that critical configurations can be demonstrated (that is, they are theoretically possible), we select a range of critical configurations. For these we use bespoke software models to understand how the critical systems could evolve as hypothetical transient criticality events and what the local physical consequences would be. Undertaking such analysis does not indicate that we consider the criticality events to be likely, or even possible. Indeed, some of the hypothetical criticality events considered are expected to have a vanishingly small likelihood of occurrence. This includes, for example, critical configurations that require hundreds of kilograms of fissile material, or those that require a large fraction of ^{239}Pu, but would take so long to develop that this is not considered credible due to the radioactive decay of ^{239}Pu.

The software models to understand the consequences of hypothetical criticality events have been developed specifically for application to 'what-if' scenarios for the GDF. The models and their application to hypothetical criticality events from the different 'what-if' scenarios are discussed further in Section 6.

4.9 The Oklo natural reactors

One set of criticality events that occurred naturally, deep underground over two billion years ago, were the Oklo natural reactors. Analysis of the Oklo natural reactors enables us to build confidence in our understanding of how critical systems might evolve.

The Oklo natural reactors were discovered in 1972 in Gabon [35,36]. Samples of uranium ore had less than the present day natural ratio of ^{235}U to ^{238}U. It was established, through various investigations and by the presence of fission products, that these samples were the result of a natural nuclear fission chain reaction. It has since been established that a number of reactor zones underwent nuclear fission about two billion years ago. At that time the fraction of ^{235}U in natural uranium was about 3.7 wt%, compared with today's value of 0.71 wt%; the half-life of ^{235}U being 704 million years. Figure 13 shows a photograph of one of the Oklo natural reactors. As one of a series of reports on natural analogues we have produced a short report that summarises our knowledge of the reactors [74].

Figure 13 A photograph showing one of the Oklo natural reactors in Gabon, Africa [74] 'reproduced with the permission of F. Gauthier-Lafaye'

Box 4 describes what we understand about the Oklo natural reactors and their implications for assessing the likelihood and consequences of a post-closure criticality in the GDF.

Box 4 The Oklo natural reactors

The believed formation and operation of the Oklo natural reactors, with indicative timescales, is summarised below.

Formation (duration ~10^7-10^8 years)

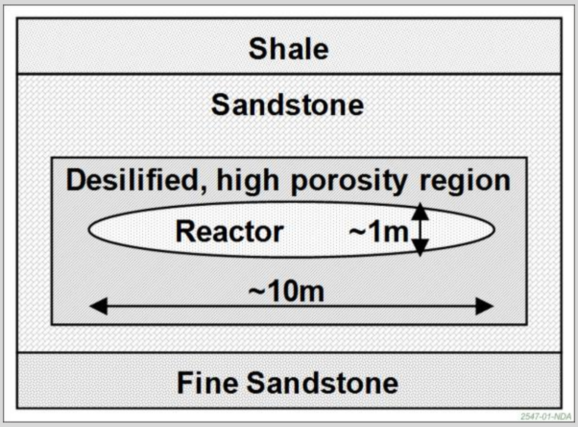
About two billion years ago, when the ratio of ^{235}U to ^{238}U was 3.7 wt% rather than the current value of 0.71 wt%, atmospheric changes led to uranium oxidation so that it was more soluble in water. The uranium was transported by water and deposited in sandstone layers at a concentration of about 0.1% to 1% uranium by mass. The layers were then covered by deep marine deposits.

Tectonic activity, fracturing and further transport of the uranium led to regions with high uranium concentrations of 15% to 60% by mass (compared with 0.2% to 0.4% in typical uranium ores). These locally high uranium concentrations led to an initial criticality and energy release from fission.

Operation (duration ~10^5 years)

The energy release from fission led to higher water temperatures and desilification of the surrounding rock, with an increased porosity of the order of 10%. The critical region expanded, while particles from desilification reduced groundwater flows.

The geometry and porosity stabilised, with the burn-out of neutron absorbers maintaining a just-critical configuration.



The reaction zones formed tended to be 'lens shaped', typically 10 m in diameter and up to 1m thick, containing tonne quantities of fissile material. The power and rate of burn-up were controlled by heat transfer to the surroundings.

After ~10^5 years the burn-up of ^{235}U and fission product poisoning ended the criticality and the reactor shut down. In the period since the reactors operated the high porosity region has been compressed under lithostatic pressure.

The Oklo natural reactors add significantly to our knowledge base by providing evidence that naturally occurring geological events can, in some circumstances, lead to the development of critical conditions. This demonstrates that, when fissile materials are present in a location that can evolve over long timescales, the likelihood of criticality may not be zero. It is noted, however, that the high enrichment of the uranium (relative to present day values), the high concentrations of uranium, the lack of sufficient neutron absorbers, and the presence of sufficient water moderator were all pre-requisites for the natural reactors. For similar conditions in the GDF, significant evolution from the sub-critical emplacement configurations would be required.

The Oklo reactors provide independent measurements for comparison with our understanding of the consequences of criticality. Boreholes and the mining of uranium have provided information on the size and geometry of the reactors and the uranium content. Measurements of fission product isotopes allow the amount of fission to be estimated, while crystallography provides information on the operating temperature. From these measurements the duration, uranium burn-up, power and fluence (number of neutrons per unit area) of the natural reactors can be estimated, without the need to undertake parameter fitting simulations. These measured and derived quantities can be compared with those from analysis using the software model we have developed to understand long-lived criticality transients (Section 6), and hence provide an important opportunity to build confidence in our modelling approach.

5 The Likelihood of a Post-closure Criticality

In this section we present the results of our research that has developed, documented and communicated the qualitative and quantitative arguments required to analyse the likelihood of post-closure criticality.

We have demonstrated that measures will be in place to ensure that criticality will not occur during the transport and operational phases of the GDF.

There is also a regulatory requirement [20] to demonstrate, as part of our Environmental Safety Case, that criticality in the GDF following closure of the facility is not a significant concern. Or to use alternative terminology, is a low likelihood event and even if one of these unlikely events was to occur over extended post-closure timescales, the consequences would be insignificant.

The detailed results of our work are presented in separate reports on LLW, ILW and DNLEU disposal [72] and SF, HLW, HEU and plutonium disposal [73] and a higher-level summary of the work is provided in an overall synthesis report [34].

In subsection 5.1 of this report we describe the methodology undertaken in the likelihood of criticality project and in subsections 5.2 and 5.3 we describe the results of the post-closure criticality scenario analysis for LLW, ILW and DNLEU and SF, HLW, HEU and plutonium disposal, respectively. Subsection 5.4 briefly discusses international experience in assessing the likelihood of criticality. Conclusions on the work to assess the likelihood of criticality are presented in subsection 5.5.

5.1 Likelihood of criticality assessment methodology

Having identified potential scenarios that could give rise to a criticality, the likelihood of a criticality has been considered by making qualitative judgements about the credibility of the scenarios, and by carrying out probabilistic modelling.

As discussed previously, a range of UK geologies is considered suitable for the GDF. We have defined three host rocks that encompass typical, potentially suitable UK geologies (higher strength rocks, lower strength sedimentary rocks and evaporites). The illustrative GDF designs for these three host rocks are based on the assumption of a single facility to accommodate all of the wastes and materials in the 2010 Derived Inventory (based on the 2007 UK RWI). In such a ‘co-located’ disposal facility it is assumed that there will be two distinct disposal areas, one for ILW, LLW and DNLEU and the other for HLW, SF, plutonium and HEU. The analysis of the likelihood of criticality in the GDF has considered the two disposal areas separately [72,73]. The concept of co-location is discussed in further detail in [4,75].

At the time of disposal, controls will ensure that all waste packages are sub-critical with substantial safety margins (see section 3). Therefore, for post-closure criticality to occur, substantial degradation and relocation of wasteform materials would be required. As discussed in section 4, understanding the radioactive waste inventories, the GDF concepts for the different waste types and host rocks, and the expected evolution of conditions in the different GDF concepts, as well as associated uncertainties, has been of fundamental importance in developing our understanding of the likelihood of post-closure criticality. These factors have been considered in order to identify criticality FEPs for each disposal concept in terms of events and processes that could result in increases in reactivity after GDF closure. Criticality scenarios have been constructed based on consideration of sequences and combinations of these criticality FEPs. As discussed in Section 4, these criticality scenarios have been defined broadly in terms of:

- FEPs that could result in increased reactivity inside a single waste package
- FEPs that could result in accumulation of fissile material outside a single waste package
- FEPs that could result in accumulation of fissile material from multiple waste packages.

These criticality scenarios have been analysed in different ways, depending on the fissile material contents of waste packages and the expected evolution of conditions in the GDF:

- if a waste package contains insufficient fissile material for criticality, even under the most favourable conditions that can be envisaged for criticality in the vicinity of the waste package, single package scale criticality is not credible.
- where such judgments cannot be made, or where scenarios involving accumulation of fissile material from more than one waste package are considered, a more detailed analysis has been undertaken of waste package degradation and fissile material relocation in order to estimate the likelihood of criticality. In this case a probabilistic modelling approach has been undertaken in which parameter value uncertainties are accounted for in probability density functions or arbitrary assumptions are made about the occurrence or otherwise of particular processes. The GoldSim Monte Carlo simulation software [32,33] has been used for this probabilistic modelling. Probability distributions have been sampled over many model runs (realisations) in order to understand the likelihood of critical concentrations or masses of fissile material developing after GDF closure.

The judgments made about the conditions required for criticality in different components of the GDF (in waste packages, engineered barriers and host rock) are important to the analysis. However, there are large uncertainties in the materials that might be involved in fissile material accumulation scenarios and the configurations of the accumulated material. In many cases, such uncertainties have been addressed by making bounding assumptions about fissile material accumulations, such as assuming that fissile material accumulates in optimal spherical or slab configurations and ignoring neutron absorbing materials that could be present. Data on minimum critical masses and concentrations of fissile material in such configurations have been used to judge whether critical systems could develop in the different components of the GDF using the above-noted deterministic and probabilistic approaches. In other cases, neutron transport calculations have been undertaken using MCNP [45] to determine whether the evolving systems evaluated using the GoldSim model remain sub-critical.

In many cases, the analysis has shown that it is not possible to accumulate a critical mass or concentration of fissile material, conditional on the treatment of parameter value uncertainty and bounding assumptions about the requirements for criticality. In other cases, the probabilistic modelling has shown that it is possible to accumulate a critical mass of fissile material, or alternatively that it is not possible to demonstrate zero likelihood (at this generic/non-site-specific stage of the programme). In these cases it is possible to make qualitative judgments about the low likelihood of criticality, again conditional on the treatment of parameter value uncertainty. However, at no point has the overall likelihood of criticality in the GDF been calculated using probabilistic models. Such an approach is not thought to be a sensible objective, particularly at the current generic phase of GDF development.

GDF post-closure criticality scenarios depend on the evolution of conditions in the near field of the GDF and/or the migration of fissile radionuclides over long time periods. A timeframe of two million years was chosen for the assessment of criticality scenarios for the GDF for LLW, ILW and DNLEU and a nominal timeframe of 100 million years was chosen for the assessment of criticality scenarios for the GDF for SF, HLW, HEU and plutonium to cover potential failure of long-lived containers due to corrosion[24]. These timeframes allow for the decay of ^{239}Pu to negligible amounts (241,000 years representing ten half-lives of ^{239}Pu) and are intended to ensure that the release of fissile material from corroded containers and its migration through the near field are represented. However, as noted in subsection 4.4, conditions in the GDF and radionuclide migration could be affected by external factors, such as climate change, which could become significant over extended post-closure timeframes. As there can be little confidence in the results of calculations this far into the future they should therefore only be regarded as indicative of likely performance beyond a few hundred thousand years.

5.2 Assessment results for LLW, ILW and DNLEU disposal

Post-closure criticality is not credible for the vast majority of LHGW packages.

In this subsection we describe the findings of our likelihood of criticality work relating to the disposal of LLW, ILW and DNLEU. We discuss the disposal of such wastes in higher strength rock, lower-strength sedimentary rock and evaporite in turn.

5.2.1 LLW, ILW and DNLEU disposal in higher strength rock

In the probabilistic modelling, criticality was calculated to be possible in a small number of realisations for specific waste packages (just under 2% of unshielded ILW packages) with a high fissile material content. Importantly, however, these packaging proposals have not yet been assessed in the Disposability Assessment process.

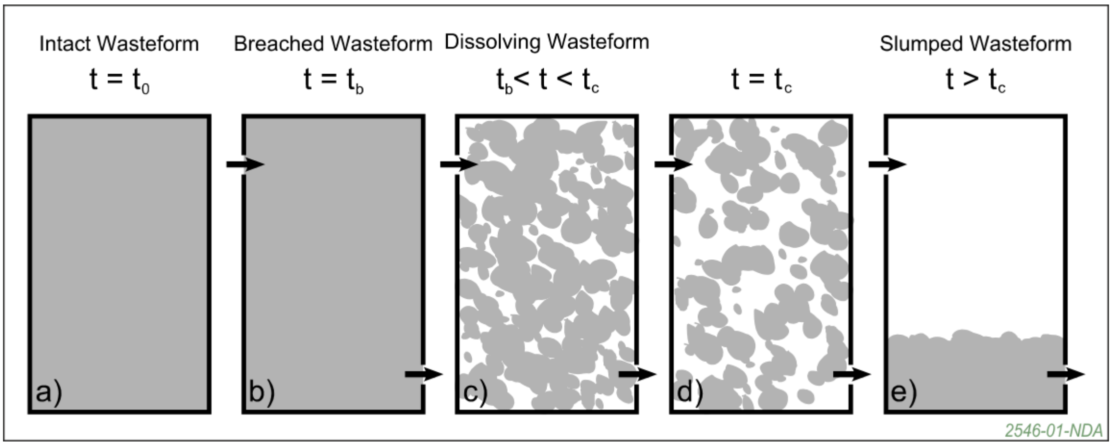
This subsection describes the findings of the likelihood of criticality work relating to the disposal of LLW, ILW and DNLEU in higher strength rock [34,72]. A conceptual model for a criticality scenario involving increases in reactivity inside a waste package is depicted in Figure 14, where it is assumed that a cementitious grout has been used to encapsulate the ILW in the container. The figure indicates: (a) an intact container at the time of GDF closure t_0 that is gradually saturating as water enters through gas vents or a package defect; (b) degradation of the container to the extent that water is able to move through the wasteform at breach time t_b (as depicted by the arrows); (c) dissolution of wasteform materials and their removal in circulating groundwater, which increases wasteform porosity and leads to some settling of remaining solids; (d) at time t_c a limiting porosity is achieved at which the remaining wasteform is assumed to be unable to support itself, leading to (e) relocation of the wasteform towards the base of the waste package. Any fissile material released from the waste package would migrate through the NRVB and potentially through seals and the host rock.

A probabilistic GoldSim model has been developed for a single waste package in order to evaluate the likely masses of plutonium, uranium and grout that remain in a waste package and the migration of uranium and plutonium from a waste package into the surrounding buffer after disposal. The effects of uncertainties in assumed parameter values have been taken into account by running the model many times (1,000), sampling different values from the parameter value distributions for each model run (realisation). Simple tests were

[24] In order to provide an indication of the potential behaviour of wastes in a copper container after failure by corrosion, the calculational timeframe was extended to 10^8 years.

conducted to confirm that 1000 realisations resulted in suitably converged results[25] (see [58] and Box 5 for further details).

Figure 14 Illustration of dissolution, settling and slumping assumed for a single LLW, ILW or DNLEU wasteform inside a disposal container (t_c = limiting porosity at which wasteform is no longer self-supporting) [72]



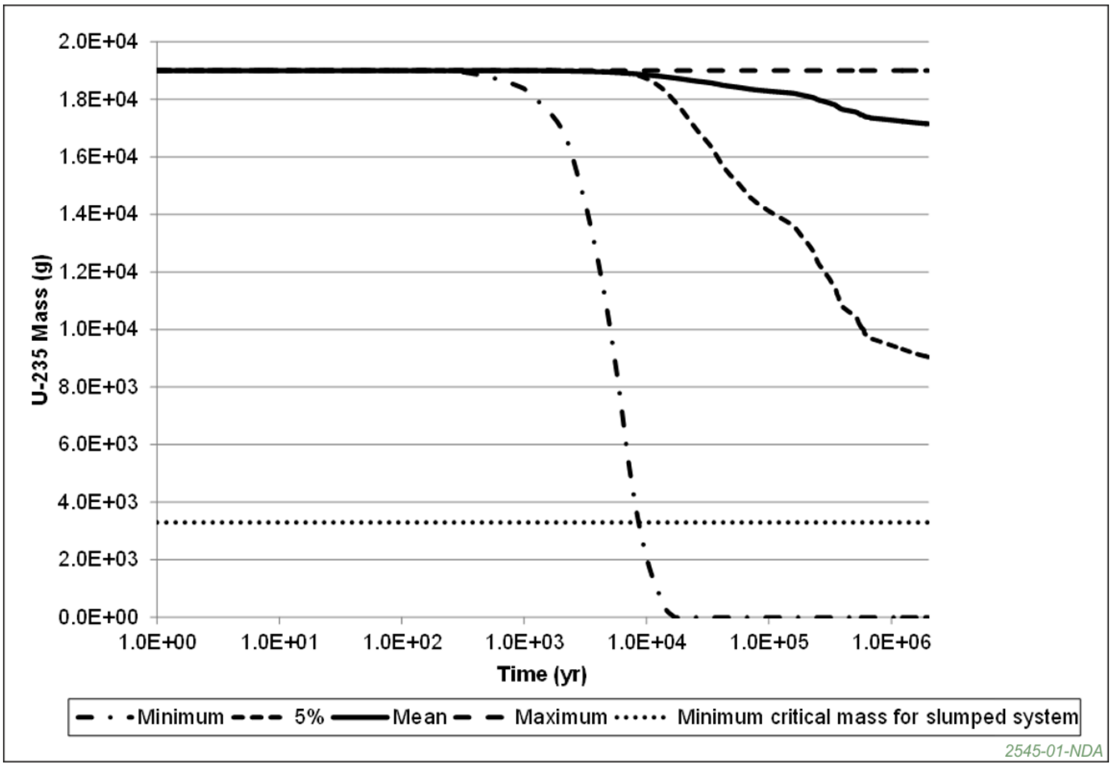
As discussed in subsection 3.4, generic CSAs have been produced for ILW packages containing highly enriched uranium (ILW-HEU) [51], low enriched uranium (ILW-LEU) [52], irradiated natural and slightly enriched uranium (ILW-INU) [53], and separated plutonium (ILW-Pu) [54]. These generic CSAs include calculations of the critical mass of fissile material that has been assumed to settle to the base of the waste package. The results of GoldSim calculations for specific ILW packages have been compared with these critical masses to determine if critical systems could form. It has been shown that the vast majority of ILW packages include (or will include) on average less than the relevant minimum masses of fissile material calculated in the generic CSAs for package-scale scenarios and, therefore, package-scale criticality is not credible for these packages.

However, it has not been possible to demonstrate that post-closure in-package criticality is impossible for all ILW packages. As an example, some model realisations for ILW packages that contain relatively high masses of LEU or HEU showed that, based on the assumed uranium solubility distribution, sufficient fissile material for criticality could be present in the waste packages even if slumping occurred on extremely long timescales. By way of an example, results for a waste package (whose design has not yet been assessed in the Disposability Assessment process) that potentially contains 19 kg ^{235}U in uranium at an enrichment of 2 wt% ^{235}U (waste stream MU006 in the 2010 Derived Inventory, based on the 2007 UK RWI[26]) are shown in Figure 15. If grout is dissolved and removed from the waste package on a timescale of a million years, then for over 95% of the realisations there would be enough uranium remaining in the waste package for criticality to occur as a result of slumping of the uranium to the base of the package. This can be observed from Figure 15 as all bar the minimum results line are significantly above the indicated minimum critical mass of 3.3 kg ^{235}U after a million years have elapsed.

[25] A probabilistic Monte-Carlo simulation is said to be converged with respect to the number of realisations carried out when further increasing the number of realisations does not significantly alter the statistics (such as the mean and standard deviation) of the output quantities.

[26] It should be noted that waste stream MU006 is no longer included in the updated 2013 Derived Inventory.

Figure 15 Example of dissolution, settling and slumping of an ILW (LEU) wasteform inside a disposal package. The critical mass of a slumped configuration for waste packages containing uranium at 4.0 wt% ^{235}U is 3.3 kg ^{235}U [52] (as indicated in the figure) and the critical mass for waste packages containing uranium at 1.9 wt% ^{235}U is 4.9 kg ^{235}U [53]. The figure is reproduced from [72]



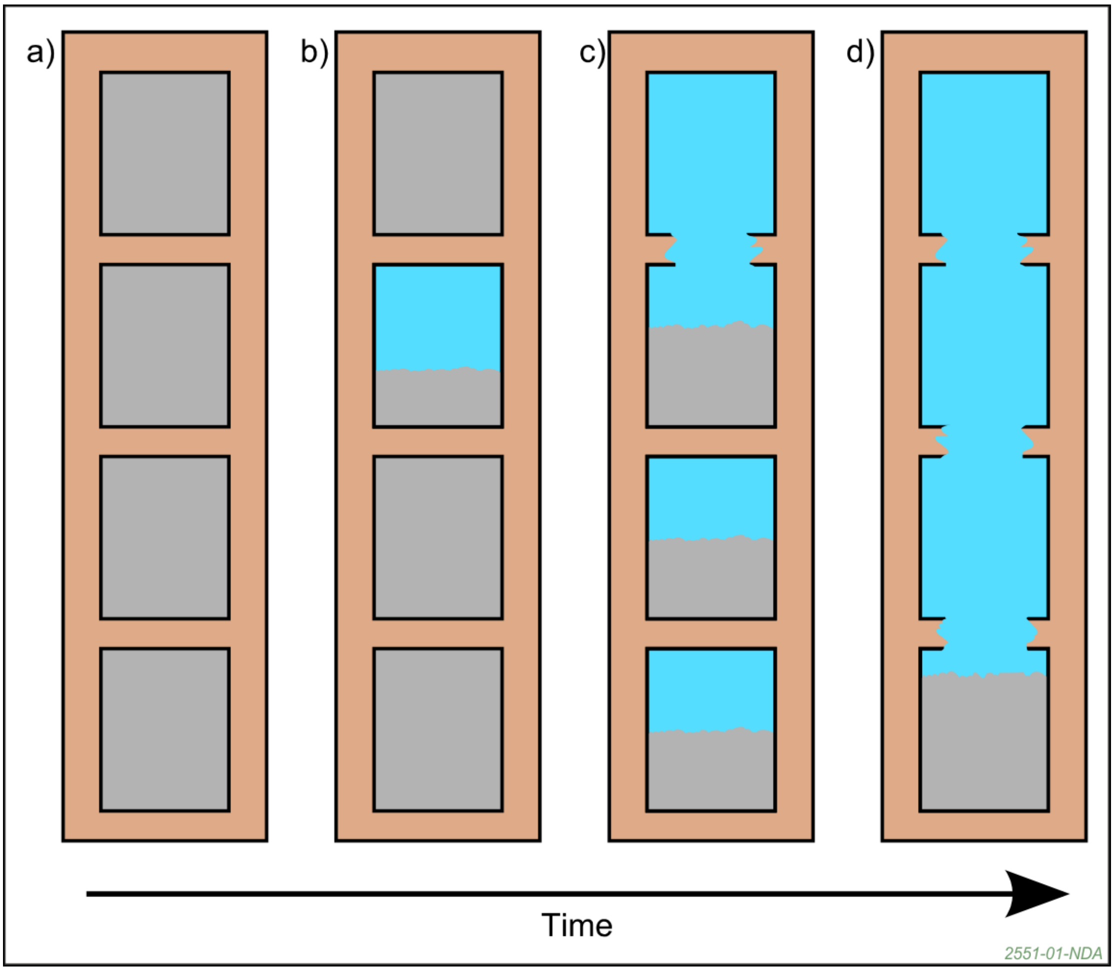
Model calculations have also indicated that conditions may not remain demonstrably sub-critical in the backfill in the vicinity of waste packages that initially contained relatively high masses of fissile material at high enrichments. This judgment has been made based on comparison of the calculated concentrations of fissile material in the backfill with minimum concentrations of fissile material required for criticality in NRVB at relevant enrichments. It should be noted that the various geochemical processes that would be required in order to mobilise the fissile materials and re-precipitate them out of solution were not factored into these scenario assessments.

The release, migration and mixing of fissile material from many waste packages could result in the generation of systems of higher reactivity than at the time of disposal. Criticality scenarios involving slumping of fissile material through a stack of degrading waste packages and accumulation of mobilised fissile material in engineered or natural barriers have been identified. These fissile material accumulation processes have been included in a single GoldSim model representing a two-dimensional (7 × 7) array of waste packages surrounded by saturated NRVB in a cross-section of a disposal vault [72].

The scenario involves progressive gravitational settling of material through a stack of waste packages as the containers corrode and wasteform and backfill materials are removed in groundwater. The process of accumulation of fissile material by slumping through multiple degraded waste packages is illustrated schematically in Figure 16. As noted previously (see subsection 4.6.1), it is not expected that significant voids would occur in an appropriately sited GDF.

In addition, uranium and plutonium could migrate from corroded waste packages and slumped systems, through the disposal vault towards the host rock, due to groundwater flow. As a result, there is also potential for mixing of fissile material from different waste packages at accumulation zones in waste packages and backfill within the ILW disposal vault, and within the surrounding host rock.

Figure 16 Illustration of the stack slumping scenario assumed for LLW, ILW and DNLEU waste packages



In the model, the package type and fissile material inventory of each of the packages in the array were selected at random. Whether the slumped systems can become critical has then been determined based on consideration of the minimum areal densities of fissile material required for criticality in water-moderated, water-reflected slabs at different enrichments[27]. Slumped material has been assumed to accumulate at the base of a unit cell, but the presence of neutron absorbing materials, such as iron corrosion products, has been conservatively ignored.

In the initial calculations, the effects of organic degradation products on uranium and plutonium behaviour were excluded. Despite the accumulation of fissile material by slumping, the minimum critical mass at the relevant enrichment was not exceeded at any location during the course of each realisation. Therefore, criticality by slumping is not credible based on the understanding of fissile material migration and accumulation processes represented in the waste package slumping analysis and assuming random

[27] This approach essentially compares the amount of fissile material in a slumped package with the limits defined in the relevant gCSAs (see [51-54]). For LEU systems the gCSA safe fissile mass calculations included consideration of a heterogeneous distribution of fuel particles in water, as such systems can be more reactive than homogeneous distributions at the assumed enrichment.

waste package inventories (the deterministic approach to set package fissile material limits explained in subsection 3.4.2 assumes that ILW stacks contain identically loaded packages from only one waste stream).

The model results show that for realisations in which the flow rate and uranium solubility are high[28], uranium can be removed from failed waste packages before slumping occurs. In such realisations, almost the entire uranium content in the vault cross-section (about 1,000 kg uranium) is transferred to the accumulation zone (the area where fissile material is assumed to gather) in one million years and the enrichment of the uranium in this zone is never more than about 1 wt% ^{235}U (that is, the average effective enrichment of the entire ILW inventory).

At the other extreme, there are also realisations for which the uranium solubility and flow rate are so low that there is little mass transfer from failed waste packages. In such cases, only a few grams of uranium reach the downstream accumulation zone on a timescale of one million years.

Critical systems could only develop if the fissile material is assumed to accumulate with water in optimum spherical configurations in porous material such as backfill. For example, in about 2% of the realisations (excluding the effects of organic material degradation products), at particular locations and times, the ^{235}U mass exceeds that required for criticality in a water-moderated sphere of ^{235}U in NRVB with a porosity of 50%. Even if all of the fissile material leaving the disposal vault cross-section accumulates in a single location (assumed to be in NRVB), the minimum critical mass under optimum conditions is exceeded in only about 2% of realisations. The conditions of concern can generally be traced back to specific waste packages (sampled at random) with a high fissile material content, which represent just under 2% of unshielded ILW packages. Importantly, these packages of ‘concern’ have not yet been assessed in the Disposability Assessment process. When they are assessed it may transpire that they do not contain as much fissile material as currently assumed, or that they may not be disposed of in the form assumed in the 2010 Derived Inventory, based on the 2007 UK RWI.

Subsequently, calculations were carried out assuming that organic material degradation products affect the migration behaviour of uranium and plutonium. In this case there is less potential for fissile material accumulation to result in criticality in the disposal vault because the increased mobility of the uranium and plutonium means that there is less available to contribute to fissile material accumulation by slumping. However, the more rapid transport of fissile material to the hypothetical accumulation zone means that there is greater potential for critical systems to develop in that (downstream) zone. For example, in many realisations, of the order 1 kg ^{239}Pu migrates to the accumulation zone. Such masses of ^{239}Pu would not be sub-critical in a water-moderated spherical configuration in NRVB. Similarly, in a number of realisations, the ^{235}U is present in the accumulation zone in masses that would not be sub-critical in a water-moderated spherical configuration in NRVB at the relevant enrichment.

If the hypothetical accumulation is assumed to occur in a low porosity (~1%) crystalline host rock, then at least 80 kg ^{235}U (in the form of UO_2) would be required for criticality under idealised conditions [76]. Such a mass of ^{235}U does not accumulate in the hypothetical accumulation zone in any realisation.

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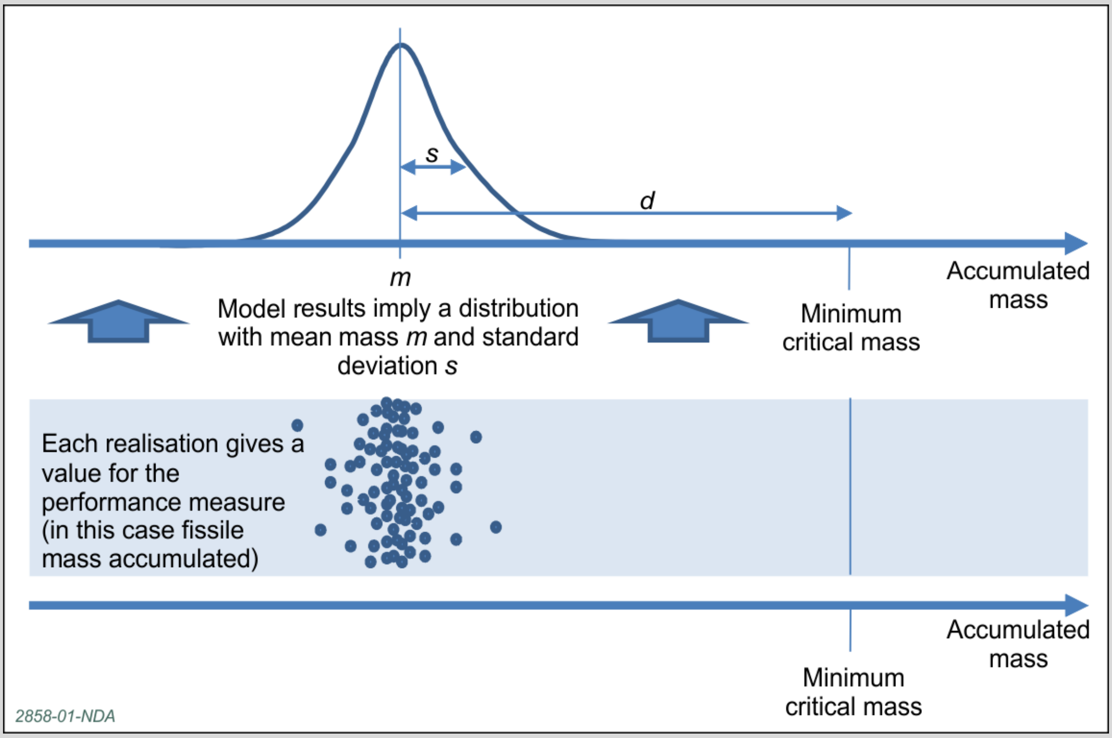
[28] It should be noted that the expected uranium solubility under high pH conditions is 1.0×10^{-4} mol/m^3. The rate of advection of uranium from a waste package would be of the order of 10^{-4} g/year, with only a few grams of uranium having been removed in 10,000 years. However, if the flux through a 500 litre drum is 10^{-1} m^3/year and the uranium solubility is as high as 10 mol/m^3 the rate of removal of uranium would be of the order of hundreds of grams per year (for further discussion on solubility see [5] and for the discussed parameter values see [9]).

It should be noted that 2% of realisations causing a critical accumulation of fissile material does not equate to a 2% likelihood or probability of post-closure criticality occurring.

Box 5 summarises what it means in terms of the likelihood (or probability) of post-closure criticality when no realisations within a thousand GoldSim modelling runs achieve a minimum critical mass.

Box 5 Interpreting GoldSim modelling results – what is the likelihood if no realisations (in 1000) achieve a minimum critical mass

The approach to interpreting probabilistic GoldSim results is illustrated below. The illustration shows what the results of the GoldSim model realisations mean in terms of the likelihood of criticality, assuming that the results at any time are normally distributed with a mean m and standard deviation σ. It is considered that 1,000 realisations are sufficient to generate the distribution. The likelihood of achieving a minimum critical mass depends on how many standard deviations the mean is from the minimum critical mass. For example, if the difference d = 3σ, then the likelihood of achieving a minimum critical mass is around 0.0014. If d = 6σ, the likelihood is about one in a billion.



5.2.2 LLW, ILW and DNLEU disposal in lower strength sedimentary rock

With no significant advection, the potential for a significant proportion of material to be removed from waste packages and slumping to occur is small. Diffusion from degraded waste packages will result in gradual migration of uranium into the backfill but conditions would remain sub-critical.

This subsection describes the findings of the likelihood of criticality work relating to the disposal of LLW, ILW and DNLEU in lower strength sedimentary rock [34,72]. Based on the assumption that there is no significant component of groundwater flow, the potential for material to be removed from waste packages in sufficient quantities for voids to be created and slumping to occur is small. Host rock creep could cause the gradual compaction of the saturated backfill and the degradation of waste packages, hence the concentration of fissile material within the package will be increased. However, waste packages that meet package-scale screening levels, as described in subsection 3.4, would remain sub-critical following compaction. This is because the analysis to derive the post-closure screening levels assumed optimum concentrations of fissile material in water, with no credit taken for the diluting or neutron-absorbing effects of other wasteform materials. Compaction could not result in higher reactivity systems than assumed in the screening level calculations.

Simple diffusion modelling indicates that the uranium concentration in a waste package would reduce by several orders of magnitude before slumping could occur (if it occurs at all), which implies that the uranium concentration would be much smaller than the minimum required for criticality following slumping. The diffusion model also shows that significant concentrations would not develop around a waste package. Therefore, criticality following diffusion of uranium from a waste package into the surrounding backfill and host rock would not occur, even for the highest loaded waste packages.

5.2.3 LLW, ILW and DNLEU disposal in evaporite

The waste packages will not become saturated and there is no potential for fissile material to be removed from waste packages. Conditions will therefore remain sub-critical.

This subsection describes the findings of the likelihood of criticality work relating to the disposal of LLW, ILW and DNLEU in evaporite [34,72]. In this analysis, the evaporite host rock is assumed to be dry. Therefore, there is no significant wasteform dissolution and no mechanism for mass transfer other than as a result of the effects of rock creep. There is no potential for fissile material accumulation outside waste packages or as a result of mixing of fissile material from multiple waste packages.

Creep could cause relatively rapid waste package compaction, which would increase the concentration of fissile material in the waste packages. However, with limited quantities of neutron moderators present and neutron absorbing materials being retained in the waste packages, the waste packages will remain substantially sub-critical.

5.3 Assessment results for SF, HLW, HEU and plutonium disposal

Post-closure criticality is possible for certain waste types in higher strength rock and lower strength sedimentary rock but only on very long timescales and when cautiously compared with conservatively derived minimum critical mass/concentration conditions.

In this subsection we describe the findings of our likelihood of criticality work relating to the disposal of SF, HLW, HEU and plutonium. We discuss disposal of such wastes in higher strength rock, lower-strength sedimentary rock and evaporite in turn.

5.3.1 SF, HLW, HEU and plutonium disposal in higher strength rock

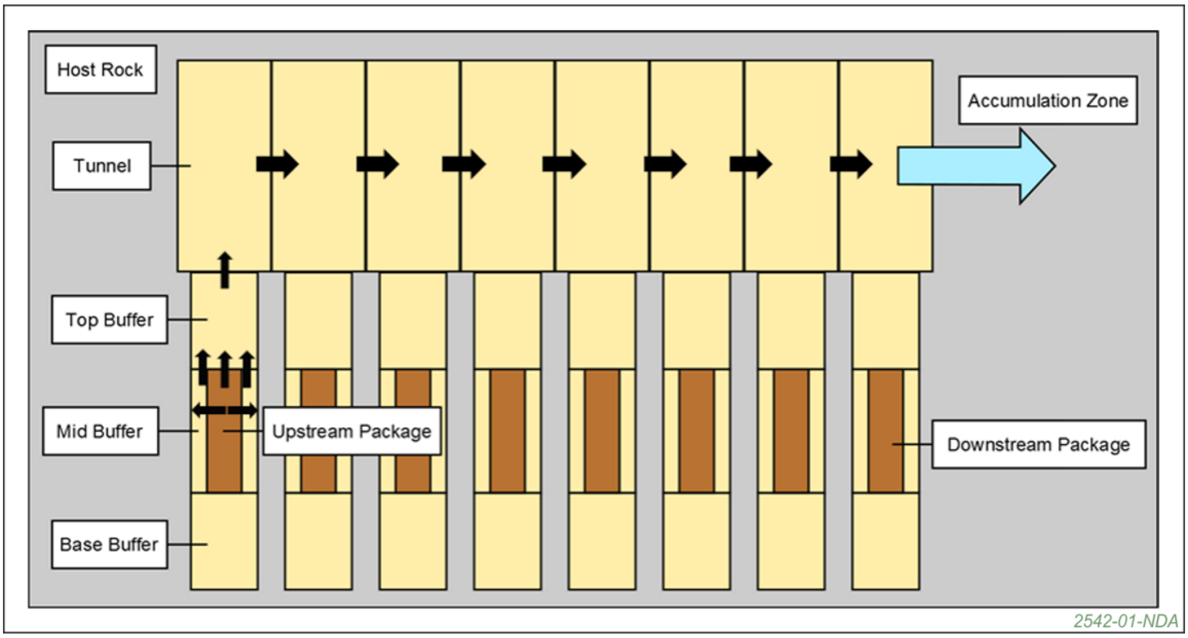
^{239}Pu will have largely decayed to ^{235}U before container failure. HLW packages contain little fissile material. Calculations show insufficient uranium would accumulate in the buffer surrounding a failed spent fuel container for criticality to occur. Sufficient ^{235}U from HEU or plutonium packages to cause a criticality could only accumulate in the buffer on very long timescales.

This subsection describes the findings of the likelihood of criticality work relating to the disposal of SF, HLW, HEU and plutonium in higher strength rock [34,73]. Consideration has been given to GDF post-closure criticality scenarios that involve rearrangement of materials in a waste package, accumulation of fissile material in the barriers outside a waste package and accumulation of fissile material from more than one waste package.

A single GoldSim model has been developed to evaluate these scenarios. The different components of the model are illustrated in Figure 17. Container failure occurs by general corrosion or by an unspecified early failure mechanism. Advective mass transfer is then assumed to occur in flowing groundwater through the waste packages and into the disposal tunnel. While the bentonite buffer around the container is present, any mass transfer from the disposal container will be by diffusion. For advective mass transfer to occur, the deposition hole would need to be close to a highly conductive fracture where the flow would be capable of eroding a substantial amount of bentonite. The layout of the disposal facility will actively avoid such intersecting zones of high hydraulic conductivity. Even so, the possibility that an accumulation zone exists downstream from a disposal region has still been considered.

Dissolved material is transferred along the disposal tunnel in flowing groundwater towards an assumed accumulation zone. No specific material properties are assigned to the downstream accumulation zone; it simply represents a void that provides a sink for all uranium and plutonium that leaves the waste packages. The accumulation zone could be interpreted as a void space in the backfill, a tunnel seal, or the host rock. The accumulation process could be interpreted as being precipitation at a location where there is a change in geochemical conditions. Mass transfer also occurs by diffusion through the buffer and backfill material and into the host rock.

Figure 17 Illustration of the components of the HLW, SF, HEU and plutonium model for the higher strength rock disposal concept [73]



To determine whether the evolving systems remain safely sub-critical requires evaluation of the neutron multiplication factor $K_{effective}$ for the systems. Neutron transport calculations were undertaken using the MCNP code to support assessments of whether the conditions within degrading waste packages remain sub-critical. The reactivity of typical backfill and tunnel materials containing fissile material that has migrated from degrading waste packages was determined from previously documented criticality calculations [95].

The neutron multiplication factor $K_{effective}$ was evaluated using MCNP for two degrading HLW, SF, HEU and plutonium package configurations:

- a configuration in which the waste package components are so degraded that the solid components have slumped to form a homogenous layer at the base of the package, with a layer of water overlying the slumped material. Uranium and plutonium are present in the slumped material and dissolved to the solubility limit in the water layer. This is the ‘segregated’ model.
- a configuration in which the material remaining in the waste package is suspended uniformly in water. This is the ‘water mixed’ model.

Calculations to evaluate the evolution and changing reactivity of HLW, SF, HEU and plutonium waste packages are presented in the following subsections. The accumulation of fissile material in the buffer, accumulation zone and surrounding host rock is also discussed.

HLW

HLW contains small amounts of fissile material. GoldSim calculations have confirmed that the reactivity of HLW packages remains low as the waste packages evolve. Most of the HLW uranium inventory is eventually transferred into the buffer material surrounding the degrading waste package, but such accumulations of ^{235}U are too small to present a criticality concern and insignificant amounts of ^{235}U are calculated to reach the tunnel or downstream accumulation zone. Accumulation of a critical mass of ^{235}U in the tunnel or host rock from multiple packages is not credible, due primarily to the fact that HLW packages include relatively small amounts of fissile material and accumulation of such material from many waste packages would be required for criticality. GoldSim calculations have indicated that, after loss of container integrity, insignificant amounts of ^{235}U are likely to migrate into any accumulation zone.

Spent Fuel

Figure 18 shows calculated material volumes in a SF package containing PWR fuel for a single typical realisation in which container failure occurs by general corrosion. Similar results have been obtained for AGR SF waste packages. The volume of copper decreases as the container corrodes until failure occurs[29]. By this time, the ^{239}Pu in the SF has decayed to ^{235}U.

After container failure, the cast iron corrodes relatively quickly, with a fraction of the iron (10%) assumed to remain in the container in the form of iron corrosion products. Most of the uranium remains in solid form, with dissolution being solubility limited. Only a small amount of dissolved uranium is advected out of the container. The MCNP water-mixed configuration results in the highest value of $K_{effective}$ (about 0.5) at the time of container failure[30]. Note that the PWR SF considered in this analysis has an effective enrichment of about 1.2 wt% ^{235}U and is therefore unsurprisingly sub-critical.

Accumulation of fissile material outside the waste package could occur in the bentonite buffer. The highest calculated ^{235}U mass in the buffer occurs in the component surrounding the PWR SF waste package (the mid-buffer component as indicated in Figure 17), but is at most little more than 1 kg ^{235}U. Such accumulations of uranium would not result in criticality even if the uranium derived from fresh PWR fuel at enrichments of a few weight percent

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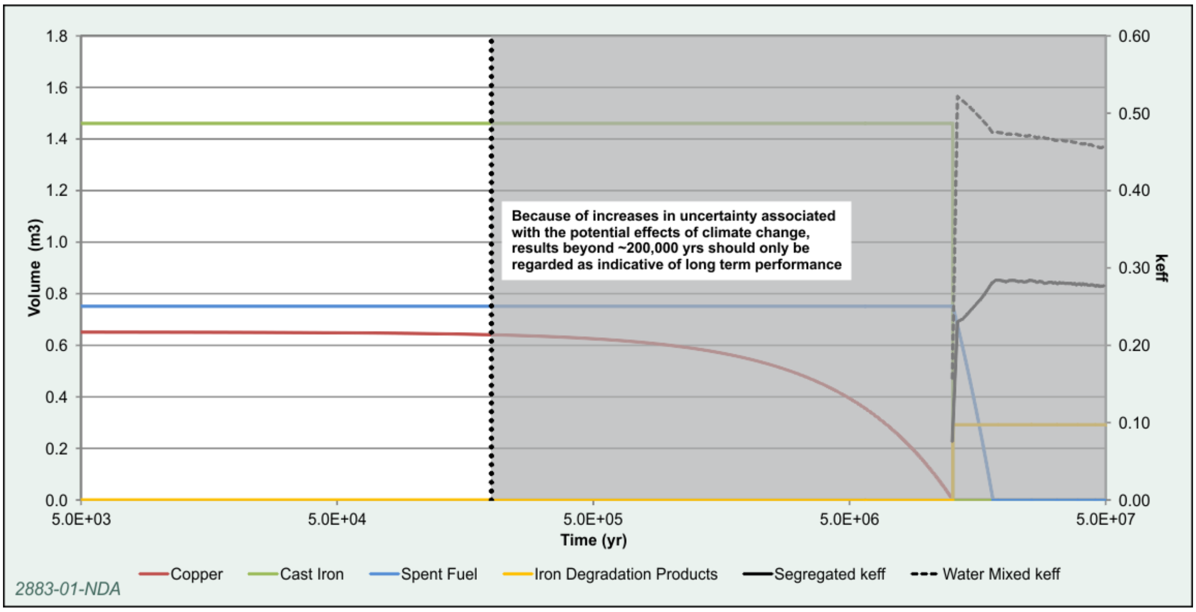
[29] Note work also considered an early container failure scenario. In the case of the HSR disposal concept this assumed that failure occurred between 200,000 and 300,000 years.

[30] It should be noted that the likelihood of criticality work (see [73]) modelled two different material relocation configurations within the SF in container scenario. A ‘segregated’ case and a ‘water mixed’ case. The two configurations were selected to represent the two extremes of possible material distributions in the waste packages. It is acknowledged that the highest reactivity conditions may occur for a configuration between the segregated and fully mixed cases.

^{235}U. A mass of at least 16 kg of ^{235}U is required for criticality in bentonite for an optimum water-moderated spherical mass of uranium dioxide at an enrichment of 3 wt% ^{235}U [95]. The calculated mass of ^{235}U in the tunnel components and downstream accumulation zone is less than 0.1 kg in the modelled period. Such accumulations of uranium would not result in criticality.

Figure 18 Predicted evolution of the volumes of package materials (left axis) and $K_{effective}$ (right axis) for a PWR SF package undergoing general corrosion. A single, typical realisation is shown [73].



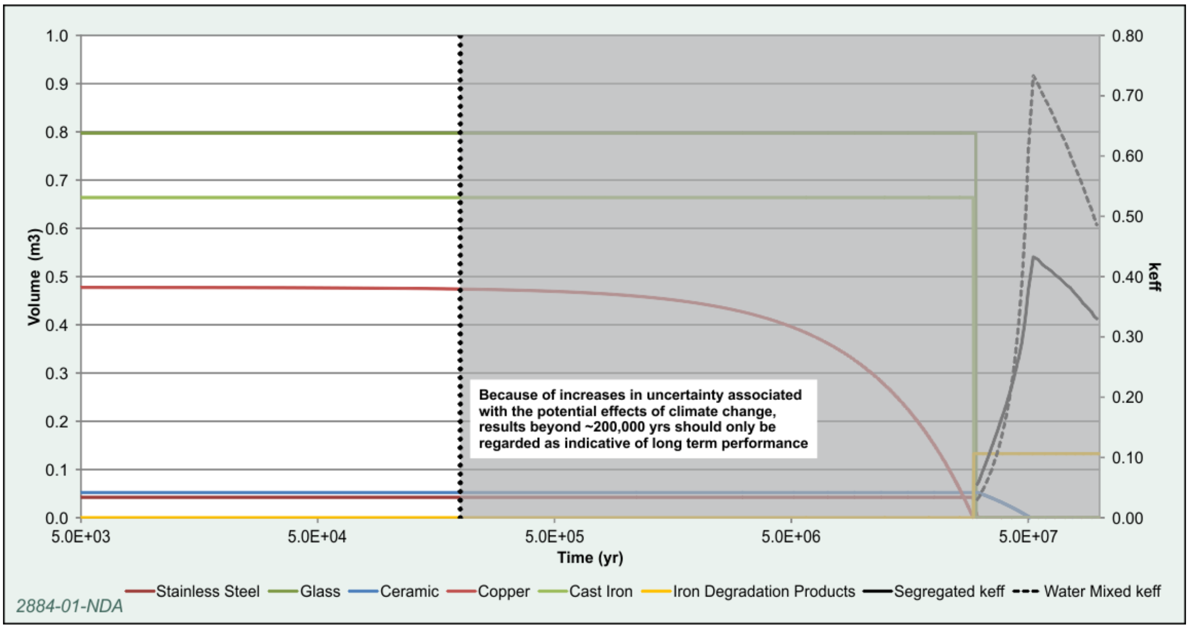
HEU/plutonium

In the case of separated plutonium waste packages, the ^{239}Pu in the package will have almost entirely decayed to ^{235}U by the time the copper container is breached by corrosion. Therefore, the results for plutonium and HEU waste packages are similar. Figure 19 shows the calculated volumes for a single realisation in which container failure occurs by general corrosion. Once the ceramic wasteform is exposed to water it begins to degrade, but most of the uranium remains in solid form for the duration of the realisation, with dissolution being solubility limited. A small amount of dissolved uranium is advected out of the container.

Cautiously, as the ceramic degrades, the neutron-absorbing materials (hafnium and gadolinium) are assumed to be dissolved and removed in the flowing groundwater. Therefore, the calculated values of $K_{effective}$ increase as the ceramic degrades, as shown in Figure 19. The water mixed configuration results in the highest value of $K_{effective}$ of about 0.75 when the ceramic has fully degraded and all of the neutron-absorbing materials have been removed. Thereafter, $K_{effective}$ decreases as the uranium is gradually dissolved and removed from the waste package.

The highest calculated uranium mass in the buffer includes about 25 kg ^{235}U and occurs in the distant future in the buffer component surrounding the HEU/plutonium waste package. The uranium has an enrichment of about 30 wt% ^{235}U (reduced from almost 100 wt% ^{235}U by the ^{238}U added to the wasteform to act as a diluent and neutron absorber). A mass of about 4 kg ^{235}U (uranium at 100 wt% ^{235}U) would be required for criticality in bentonite under optimum conditions for criticality [95]. Therefore, the model shows it is possible that criticality could occur in the buffer on timescales in excess of a million years. The mass of ^{235}U in the tunnel components and downstream accumulation zone is calculated to be less than about 3 kg in the simulation period (that is, slightly less than the above-noted critical mass of 4 kg ^{235}U).

Figure 19 Predicted evolution of the volumes of package materials (left axis) and $K_{effective}$ (right axis) for an HEU/plutonium package undergoing general corrosion. A single, typical realisation is shown [73].



5.3.2 SF, HLW, HEU and plutonium disposal in lower strength sedimentary rock

It is expected that most ^{239}Pu will have decayed to ^{235}U before significant accumulation can occur. Enough ^{235}U could accumulate in the buffer surrounding a failed PWR container to challenge the minimum critical mass in bentonite if the accumulated uranium were to derive from fresh PWR fuel.

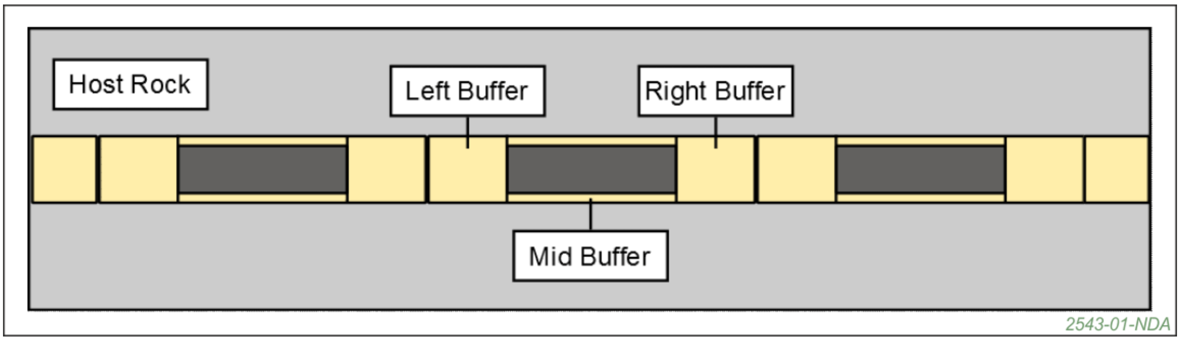
This subsection describes the findings of the likelihood of criticality work relating to the disposal of SF, HLW, HEU and plutonium in lower strength sedimentary rock [34,73]. The conceptual model for the scenario involving increases in reactivity inside a waste package is similar to that described for the GDF in higher strength host rock, except that the disposal packages are emplaced horizontally rather than vertically. However, based on the assumption that there is no significant component of groundwater flow, such that mass transfer is diffusion-dominated, the potential for material to be removed from waste packages is small.

A GoldSim model has been developed to evaluate the behaviour of degrading waste packages for the lower strength sedimentary rock disposal concept. The different components of the model are shown in Figure 20. Diffusive mass transfer is assumed to occur from failed waste packages into surrounding bentonite in the disposal tunnel. Mass transfer also occurs by diffusion from the bentonite into the host rock.

Neutron transport calculations were undertaken using MCNP to determine whether the evolving systems remain sub-critical. Two degrading HLW, SF, HEU and plutonium package configurations (the segregated case and the water-mixed case) were evaluated. Changes in package reactivity as materials migrate from the waste packages were evaluated for these configurations. The reactivity of tunnel materials and host rock containing fissile material that has migrated from degrading waste packages was determined from previously documented criticality calculations [95].

Calculations to evaluate the evolution and changing reactivity of HLW, SF, HEU and plutonium waste packages are presented in the following subsections. The accumulation of fissile material in the tunnel buffer and in the surrounding host rock is also discussed below.

Figure 20 Illustration of the components of the HLW, SF, HEU and plutonium model for the lower strength sedimentary rock disposal concept [73]



HLW

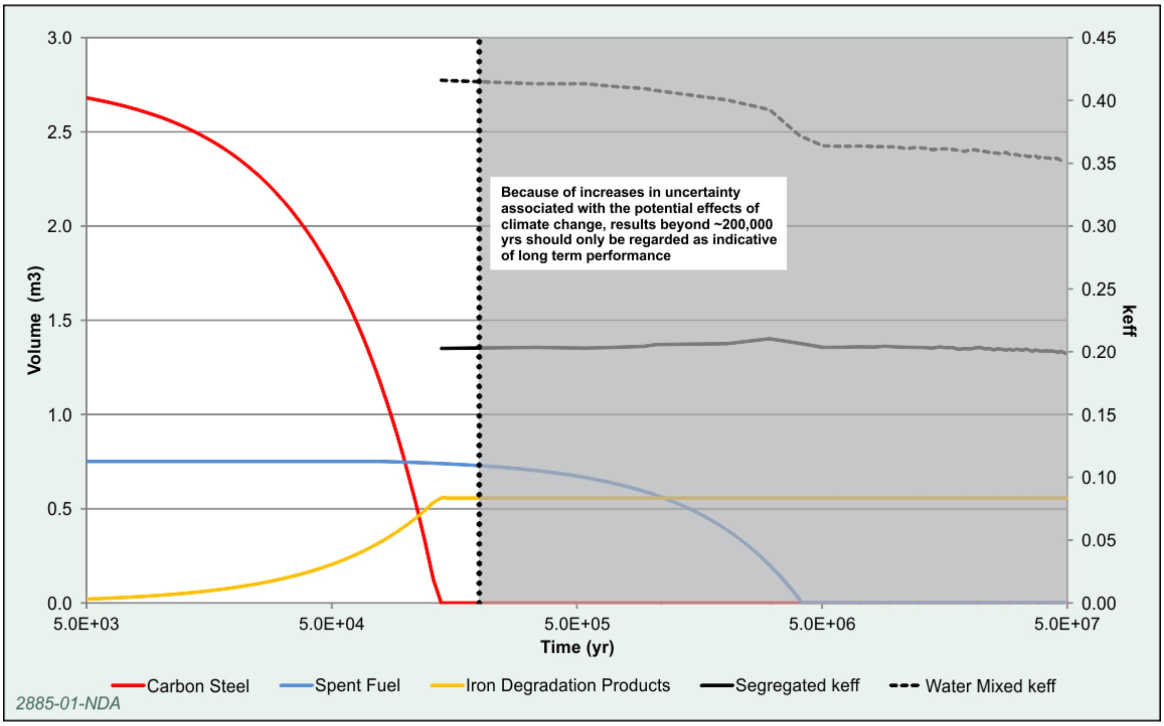
As previously noted, HLW contains only a small quantity of fissile material. Calculations have confirmed that the reactivity of HLW packages remains low as the waste packages evolve. Most of the HLW uranium inventory is eventually transferred into the buffer material surrounding the degrading waste package, but such accumulations of ^{235}U are too small to present a criticality concern and insignificant amounts of ^{235}U are calculated to reach the tunnel or downstream accumulation zone. Accumulation of a critical mass of ^{235}U in the tunnel or host rock from multiple packages is not credible.

Spent Fuel

Figure 21 shows the calculated volumes in a PWR SF waste package for a typical single realisation in which container failure occurs by general corrosion. Similar results have been obtained for AGR SF waste packages. The volume of carbon steel decreases as the container corrodes until failure occurs; an arbitrary 10% of the iron in the steel is assumed to remain in the container in the form of iron corrosion products. Most of the SF remains in solid form for the duration of the realisation, with dissolution being solubility limited. The water mixed configuration results in the highest value of $K_{effective}$ of about 0.4 after container failure. Broadly speaking, as the wasteform degrades and the uranium is transported into the buffer the reactivity of the waste package decreases.

The highest calculated mass of 20 kg ^{235}U occurs in the buffer component surrounding the waste package after over one million years. Such an accumulation of uranium would not result in criticality for PWR SF at typical fuel burn-ups. However, if the uranium derived from fresh PWR fuel at enrichments of a few weight percent ^{235}U, the calculated mass in the buffer is of the same order of magnitude as the minimum required for criticality (16 kg of ^{235}U in UO_2 in bentonite at an enrichment of 3 wt% ^{235}U [95]), although this would require the uranium to accumulate in an optimum water-moderated spherical configuration, which is a conservative assumption. The greatest mass in the host rock is 8 kg ^{235}U, which occurs at the end of the simulation period. About 600 kg ^{235}U in UO_2 at 3 wt% ^{235}U would be required for criticality in a typical sedimentary rock [95] and therefore criticality in this host rock is not credible.

Figure 21 Predicted evolution of the volumes of package materials (left axis) and $K_{effective}$ (right axis) for a PWR SF package undergoing general corrosion in the lower-strength sedimentary rock concept. A single, typical realisation is shown [73].

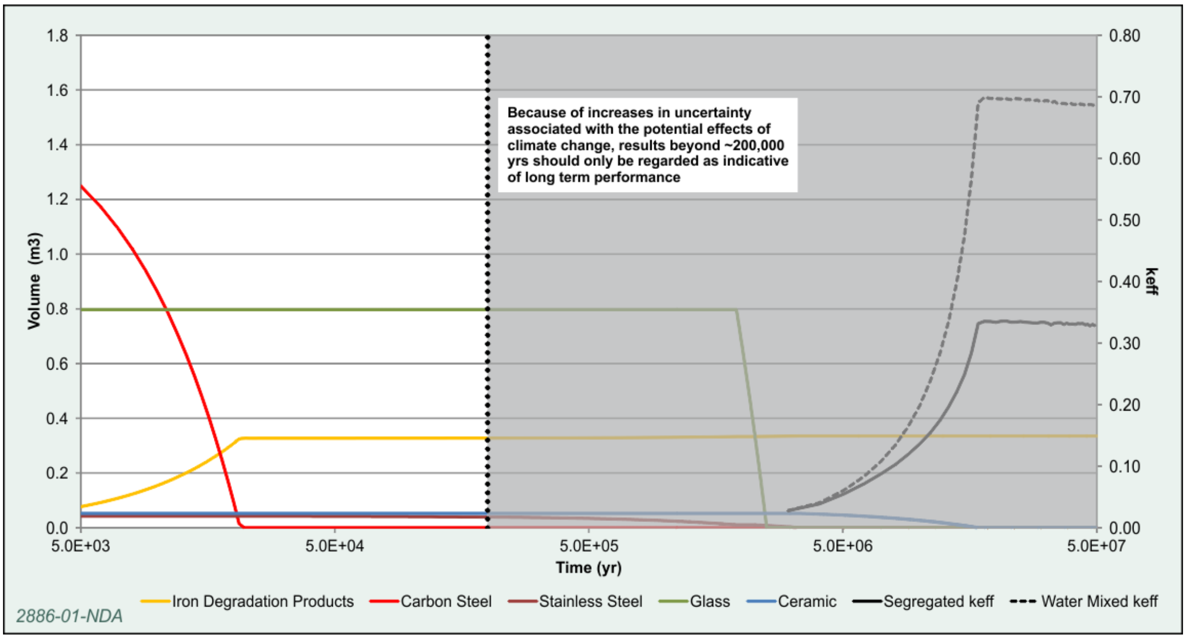


HEU and plutonium

Figure 22 shows the calculated volumes for a single realisation of an HEU waste package in which container failure occurs by general corrosion. Once the ceramic wasteform is exposed to water it begins to degrade, but most of the uranium remains in solid form for the duration of the realisation, with dissolution being solubility limited. As for the higher strength rock model, the neutron absorbing materials (hafnium and gadolinium) are assumed to be dissolved and removed in the groundwater as the ceramic degrades. Therefore, the calculated values of $K_{effective}$ increase as the ceramic degrades, as shown in Figure 22. The water mixed configuration results in the highest value of $K_{effective}$ of about 0.7 when the ceramic has fully degraded and all of the neutron-absorbing materials have been removed. Thereafter, $K_{effective}$ decreases as the uranium is gradually dissolved and removed from the waste package.

The highest calculated uranium mass includes about 25 kg ^{235}U and occurs well after a million years in the buffer component surrounding the HEU/plutonium waste package. The uranium has an enrichment of about 30 wt% ^{235}U (reduced from almost 100 wt% ^{235}U by the ^{238}U added to the wasteform to act as a diluent and neutron absorber). A mass of about 4 kg ^{235}U (uranium at 100 wt% ^{235}U) would be required for criticality in bentonite under optimum conditions for criticality [95]. Therefore, it is possible that criticality could occur in the buffer, but on timescales in excess of a million years. The greatest mass in the host rock is calculated to be about 30 kg ^{235}U at the end of the simulation period. About 5 kg ^{235}U (100 wt% ^{235}U) would be required for criticality in a typical sedimentary rock [95]. Therefore a critical mass could be generated in the host rock that exceeds the minimum critical mass calculated assuming the optimum configuration for criticality.

Figure 22 Predicted evolution of the volumes of package materials (left axis) and $K_{effective}$ (right axis) for an HEU package undergoing general corrosion in the lower strength sedimentary rock concept. A single, typical realisation is shown [73].



5.3.3 SF, HLW, HEU and plutonium disposal in evaporite

Creep of the host rock may reduce void space in waste packages, increasing fissile material concentrations, but neutron-absorbing material will be retained, eliminating the potential for criticality.

This subsection describes the findings of the likelihood of criticality work relating to the disposal of SF, HLW, HEU and plutonium in evaporite [34,73]. Again, the evaporite host rock is assumed to be dry. Therefore, there is no significant wasteform dissolution and no mechanism for mass transfer, other than as a result of the effects of rock creep. There is no potential for fissile material accumulation outside waste packages or as a result of mixing of fissile material from multiple waste packages.

Creep will cause waste package compaction, although the waste packages would be designed to resist such compaction. Compaction will increase the concentration of fissile material in the waste packages as any void space is reduced. However, with limited quantities of neutron moderators present and neutron absorbing materials being retained in the waste packages, the waste packages will remain substantially sub-critical.

5.4 International experience in assessing the likelihood of criticality

We have reviewed international approaches to understanding and demonstrating the likelihood of post-closure criticality and have sought to incorporate this understanding into the UK work programme. Where comparions could be made, the results of our work were broadly found to be consistent with other international studies.

In this section we summarise a review that we conducted on the various approaches used internationally to assess the likelihood of criticality in the GDF [34]. We focus on the identification of post-closure criticality scenarios and the methods used to assess the probability of their occurrence.

The following are selected for discussion because they aim to assess the probability of GDF post-closure criticality safety based on consideration of a comprehensive range of post-closure criticality scenarios:

- the recently published draft Criticality Safety Standard for nuclear fuel disposal in Germany [77]. This sets out the approach to be taken in addressing criticality safety for the operational and post-closure phases of a geological disposal facility. Key features of the approach to post-closure criticality safety set out in the safety standard are:
    - the safety analysis for the post-closure phase must ensure that the chances of a criticality excursion under a given scenario and, if necessary, the consequences of a postulated criticality excursion, are sufficiently limited
    - the tolerable probability of criticality is set higher for the post-closure phase (at 10^{-4}) than for the operational phase (at 10^{-6}), with a gradual increase of the limit over a transition time related to the uncertainty of the probability estimation for a given scenario.
- criticality safety assessments for radioactive waste disposal in the US, covering SF, plutonium, HLW, HEU and transuranic waste [78,79], in which the broad approach was to:
    - develop post-closure criticality scenarios
    - develop deterministic models to evaluate performance measures
    - include statistical analysis of uncertainties (which generally requires many runs of a deterministic model)
    - calculate minimum critical masses to use as safety standards to which the performance measures can be compared.
- a criticality safety assessment for SF disposal in Sweden, published in the 1970s [80], which involved detailed consideration of criticality scenarios. These scenarios comprised events and processes that could lead to criticality in a disposal container and criticality in components of the engineered barrier system and host rock. The assessment involved deterministic analysis of the processes that could lead to criticality and then neutron transport calculations to evaluate critical masses and concentrations in different configurations and media. However, the assessment did not go so far as to evaluate the probability that the criticality scenarios would occur. Instead, judgments were made that the critical systems were extremely unlikely to develop.

Other studies identified as having addressed GDF post-closure criticality have focussed on the evaluation of package-scale scenarios, and have made qualitative judgements about the potential for criticality following waste package degradation and fissile material migration and accumulation. For example:

- Wantz *et al.* [81] reported calculations to evaluate the reactivity of the Belgium SF supercontainer in the long term under disposal conditions, including disruption of the supercontainer allowing water entry, followed by loss of container fill materials (sand) and rearrangement of SF assemblies.
- Gmal *et al.* [82] presented the results of criticality analyses for the disposal of SF and fissile wastes in a clay host rock in Germany. Only package-scale scenarios were analysed, on the assumption that long range transport of dissolved fissile

material through the low-permeability rock and subsequent mixing of material from several packages would not occur.

- post-closure criticality in a geological disposal facility for SF of a specified burn-up in Sweden was judged to be unlikely in the SR-Site licence application [83]. It is stated that the risk of criticality as a result of redistribution of material has been analysed by Behrenz and Hannerz [80] and by Oversby [84,85]. The conclusions were that criticality outside the container has a vanishingly small probability, requiring several highly improbable events to occur.

5.5 Conclusions and key assumptions

We have made assessments of the likelihood of post-closure criticality. In many scenarios criticality has been shown not to be credible. The results of the analysis are conditional on a number of important assumptions.

Box 6 summarises the assessment results for the likelihood of LLW, ILW and DNLEU disposal causing post-closure criticality in the GDF.

Box 6 Summary of the likelihood of LLW, ILW and DNLEU disposal causing post-closure criticality

Disposal in a higher strength rock concept:

- post-closure criticality is not credible for the vast majority of ILW packages
- conditions required for criticality were calculated to be met in only about 2% of the probabilistic realisations for the higher strength rock disposal concept
- the conditions of concern can generally be traced back to specific waste packages with a high fissile material content, which represent just under 2% of unshielded ILW packages and importantly whose designs have not yet been assessed in the Disposability Assessment process (they may well no longer be a concern once they have).

Disposal in a lower strength sedimentary rock concept:

- there is assumed to be no significant component of groundwater flow in the lower strength sedimentary rock analysis, so that the potential for material to be removed from waste packages in sufficient quantities for voids to be created and slumping to occur is small
- diffusion from degraded waste packages will result in gradual migration of uranium into the backfill and conditions will remain sub-critical.

Disposal in an evaporite concept:

- there is assumed to be no unbound water present in the evaporite host rock, so that the waste packages will not become saturated and there is no potential for fissile material to be removed from waste packages, therefore conditions will remain sub-critical.

Box 7 summarises the assessment results for the likelihood of SF, HLW, HEU and plutonium disposal causing post-closure criticality in the GDF.

Box 7 Summary of the likelihood of SF, HLW, HEU and plutonium disposal causing post-closure criticality

Disposal in a higher strength rock concept:

- copper disposal containers are expected to maintain their integrity and containment for at least 10^5 years. Therefore, it can be expected that ^{239}Pu will have largely decayed to ^{235}U before container failure.
- HLW packages include relatively small amounts of fissile material. Accumulation of such material from many waste packages would be required for criticality. Calculations have indicated that, even after loss of container integrity, insignificant amounts of ^{235}U are likely to migrate into any accumulation zone.
- SF of the assumed burn-up will always be sub-critical under water-moderated conditions[31]. The calculations indicate that insufficient uranium for criticality would accumulate in the buffer surrounding a failed SF container.
- calculations indicate that failed HEU/plutonium packages would remain sub-critical because of the neutron absorbing components of the wasteform. Sufficient ^{235}U from HEU/plutonium packages could accumulate in the surrounding buffer to support criticality on timescales in excess of 10^6 years, although the accumulated masses have been compared with the critical masses of idealised spherical configurations, which are not considered to occur naturally and may be overly cautious.
- it should be noted that there can be limited confidence in the results of calculations into the very distant future and results should therefore be regarded only as being indicative of performance beyond a few hundred thousand years.

Disposal in a lower strength sedimentary rock concept:

- wasteform degradation rates are expected to be slow and mass transfer is expected to be diffusion-dominated. As such, it can be expected that ^{239}Pu will have decayed to ^{235}U before any significant fissile material accumulation can occur.
- however, shorter container lifetimes have been assumed for the carbon steel containers than for copper containers. As a result, in the far distant future, greater masses of uranium are calculated to migrate into the buffer surrounding a failed carbon steel container than that surrounding a copper container.
- in particular, the modelling indicates that enough ^{235}U could accumulate in the buffer surrounding a failed PWR container to challenge the minimum critical mass in bentonite (when compared to an idealised water-moderated spherical configuration, which is not considered to occur naturally) if the accumulated uranium derives from fresh PWR fuel.

Disposal in an evaporite concept:

- the evaporite host environment has been assumed to be dry, such that there is no significant wasteform dissolution and no mechanism for mass transfer other than as a result of the effects of rock creep. Creep of the host rock may reduce void space in waste packages, increasing fissile material concentrations, but neutron-absorbing material will be retained, removing the potential for criticality.

[31] Whilst this is considered to be a key likelihood argument, the justification for this resides in our static, in package criticality consequences work. This work is presented later in subsection 6.3.3.

The analysis of the likelihood of criticality following LLW, ILW and DNLEU disposal has been based on some assumptions about the waste inventory, waste packaging concepts, disposal facility design, barrier system properties and GDF evolution. Key assumptions in the analysis of LLW, ILW and DNLEU in higher strength rock are as follows:

- we assumed that the wastes were packaged as described in the 2010 Derived Inventory (based on the 2007 UK RWI) and a number of waste packages will have a high fissile material content. However, we have assessed few such waste packaging concepts through application of our Disposability Assessment process. If reductions in the fissile material content of the high fissile content waste packages were required as a result of this process, this could have a significant impact on the criticality scenario analysis.
- an important assumption made in the criticality-scenario analysis is that slumping of fissile material through voids can occur in waste packages following dissolution of the waste encapsulation grout. However, as noted in subsection 4.6.1, there may be little potential for void formation under expected geochemical and hydrological conditions. This means that assumptions made about grout dissolution rates may be cautious rather than realistic and post-closure criticality scenarios involving fissile material slumping may not in fact be credible.
- the uranium and plutonium inventory in each waste package has been selected randomly. However, waste packages could be emplaced in campaigns, such that a random distribution is not representative. If a number of similar waste packages with high fissile material content are assumed to be emplaced together, then the accumulated masses of fissile material (such as from slumping) may be significantly greater than those calculated in this analysis. For further discussion of the consideration of the waste package receipt schedule at the GDF and its potential impact on vault stacking and associated fissile material loadings, see [58].
- alternative approaches to waste packaging (potentially involving vitrification, non-encapsulation or immobilisation in polymers) have been, and may be, proposed by waste producers for some wastes; the post-closure performance of such waste packages may be substantially different to the behaviour assumed for the grouted waste packages considered in the likelihood of criticality analysis.

The most important assumption made in this analysis of LLW, ILW and DNLEU in lower strength sedimentary rock is that mass transfer is diffusion-dominated and the main assumption for LLW, ILW and DNLEU disposal in evaporite is that the host rock is dry.

The analysis of the likelihood of criticality following SF, HLW, HEU and plutonium disposal has been based on some assumptions about the waste inventory, waste packaging concepts, disposal facility design, barrier system properties and GDF evolution. Key assumptions in the analysis of SF, HLW, HEU and plutonium in higher strength rock are as follows:

- typical fuel enrichments and burn-ups have been assumed. Fresh and low burn-up fuels are likely to have higher reactivity under conditions represented by the post-closure scenarios considered in the analysis [38, 95]. The inclusion of fission products for irradiated fuels in the MCNP analysis (currently ignored) may reduce calculated reactivity.
- a ceramic wasteform and can-in-canister approach has been assumed for HEU and plutonium disposal. Alternative immobilisation matrices and packaging concepts may be used. The rates of degradation and release of fissile radionuclides from alternative immobilisation matrices and different containers may differ from those considered in this project, which would affect the potential for fissile material accumulation post-closure.

- calculations of the neutron multiplication factor for in-package scenarios have involved specific assumptions about material behaviour (for example, dissolution and removal of iron and neutron absorbing materials in groundwater). However, analysis of the behaviour of iron corrosion products under disposal conditions has indicated that iron would remain in solid form for long periods under disposal conditions. Also, the presence of the neutron absorbers hafnium and gadolinium in the degraded and accumulated material could be considered for HEU and plutonium wastes. The inclusion of greater amounts of iron and neutron absorbing materials would reduce calculated reactivity.

The most important assumption made in this analysis of SF, HLW, HEU and plutonium in lower strength sedimentary rock is that mass transfer is diffusion-dominated and the main assumption for SF, HLW, HEU and plutonium disposal in evaporite is that the host rock is dry.

It is important to acknowledge that the likelihood of post closure criticality work has been based on the 2010 Derived Inventory (itself based on the 2007 UK RWI). A significant addition to the updated 2013 Derived Inventory [39] is the inclusion of MOX SF which will be of higher enrichment, but also likely higher burn-up. Future work is planned (see [10] task 116) to look at the sensitivity of the overall likelihood of post-closure criticality conclusions to this additional fuel type. Changes associated with the ILW proportion of the inventory are considered to be less significant (in terms of criticality safety).

6 Consequences of Post-closure Criticality

In our consequences of post-closure criticality work we consider the 'what-if' scenario of sufficient accumulation of fissile materials occurring in an evolving GDF to give rise to a criticality. This is in accordance with regulatory guidance [20] and part of the assessment of the robustness of the GDF to low likelihood events (such as a post-closure criticality).

We have developed models to predict the consequences of criticality. Application of these models helps us to understand and bound the physical consequences, should such a low likelihood event occur (on extended post-closure timeframes).

The background to the 'Understanding Criticality under Repository Conditions' (UCuRC) programme and the identification of the types of criticality that might arise are summarised in subsection 6.1, which also summarises relevant evidence from known criticality events. The models developed for the programme are summarised in subsection 6.2 and recent research on assessing the consequences of criticality is described in subsection 6.3. Subsection 6.4 discusses international experience in assessing the consequences of criticality and a summary is presented in subsection 6.5.

6.1 Types of criticality

In a quasi-steady state criticality an increase in temperature causes a decrease in the reactivity of the fissile material (negative temperature feedback). This is a relatively low power criticality process which may be sustained over long timescales. In a rapid transient criticality, an initial increase in temperature causes an increase in reactivity (positive temperature feedback). This would be a higher power event with a duration of less than a second.

In the 1998 assessment of the features, events and processes that might lead to a post-closure criticality for ILW in a higher strength host rock disposal facility[32] it was concluded that, although a criticality would not be expected based on best-estimate data, the possibility of a criticality could not be entirely discounted [86].

In these circumstances we initiated the UCuRC programme, to obtain a better understanding of the processes that would control the nature and magnitude of a post-closure criticality from disposed ILW. The UCuRC programme involved the development and benchmarking of models that predict the evolution of critical systems, including the effects on the surroundings. Coupled with knowledge of the transport of radionuclides within and from the vicinity of the disposal facility, these models can be used to predict the consequences of a criticality. The detailed results of the UCuRC programme have been published in a number of technical reports as the models have been developed. A summary of the models and the associated verification, validation and benchmarking activities is given in [30]. References to the other technical reports are also given in [30].

In the unlikely event that enough fissile material is brought together by some mechanism, the chain reaction can lead to two types of criticality that have significantly different timescales and potential consequences.

In a quasi-steady state (QSS) criticality, an increase in temperature causes a decrease in the reactivity of the fissile material (a response characterised by a 'total negative temperature feedback coefficient'). Assuming that further fissile material is still accumulating (or further reactivity insertion is occurring), this allows a steady-state to be

32 The consideration of ILW disposed of in HSR was in line with the remit of Nirex. The current RWM remit extends to additional waste-streams, materials and geologies.

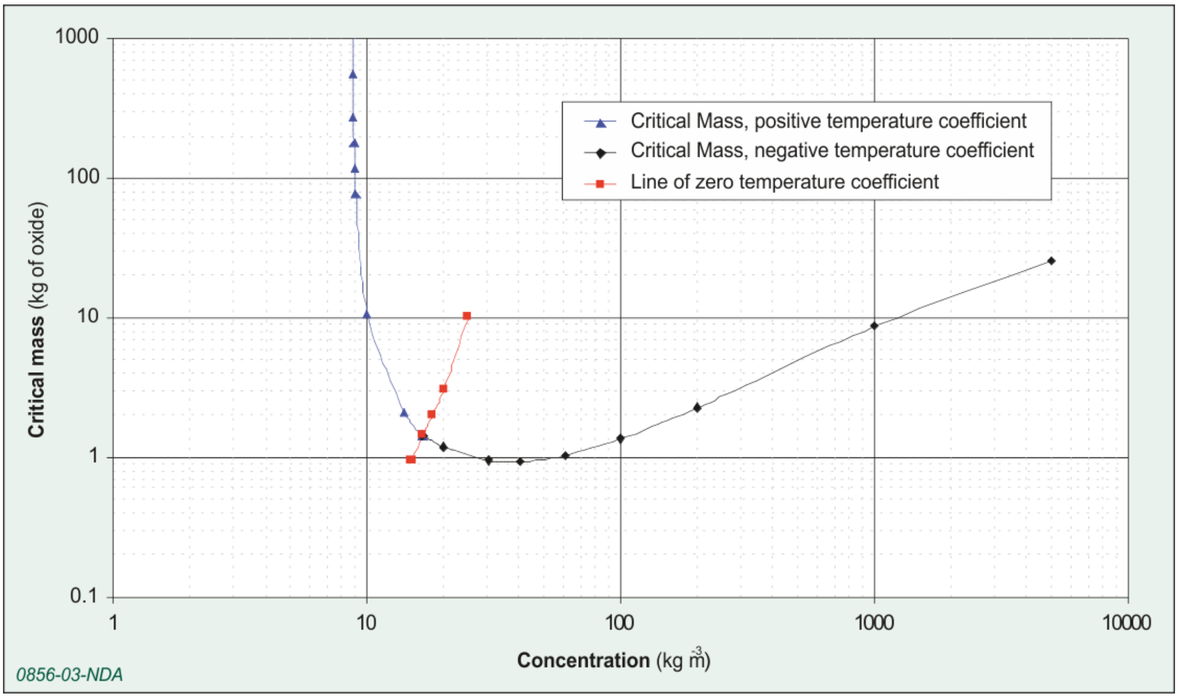
reached, often with a modest rise in temperature, in which a ‘just-critical’ configuration is maintained. This just-critical configuration could last for many millennia, such as occurred at Oklo (see Box 4). Eventually, either fissile material stops accumulating, in which case the power from the criticality will gradually decay to zero, or the burn-up is such that the ‘just-critical’ state cannot be maintained at the ambient temperature and the criticality ceases.

In a rapid transient (RT) criticality, an initial increase in temperature causes an increase in the reactivity (a response characterised by a ‘total positive temperature feedback coefficient’). In these circumstances it is not possible to maintain a ‘just-critical’ configuration, so the neutron flux and power rise lead to an escalating temperature. It is possible that the rapid transient will terminate at a relatively low temperature, if further increases in temperature decrease the reactivity. If this is not the case, then the temperature and pressure in the critical region will rise. At some point the pressure will become sufficient to drive the expansion of the critical region, leading to possible damage to the surroundings. This expansion would eventually be sufficient to terminate the criticality. The timescale for a rapid transient event is typically less than one second.

Calculations with reactor physics and criticality numerical models, similar to those used to determine the parameters for a critical system, as in Figure 10, can be used to determine whether the reactivity of a system increases or decreases with temperature (the total temperature feedback of the system). Results for an accumulation of ^{239}Pu in saturated backfill are shown in Figure 23 [70]. This shows that if the criticality were to occur at a plutonium dioxide concentration of less than ~16 kg/m^3 (to the left of the red line of zero temperature coefficient), then the total temperature feedback would be positive and so a rapid transient criticality would occur. However, at higher plutonium dioxide concentrations, outside of the very narrow, low concentration total positive temperature feedback range, (to the right of the line of zero temperature coefficient), the total temperature feedback is always negative, so only a quasi-steady state criticality could result. ^{235}U systems lead to a quasi-steady state criticality, rather than a rapid transient, in almost all circumstances [38].

Our static criticality work has thus far focused on accumulations of ^{235}U and/or ^{239}Pu, as these are by far the two most abundant fissile radionuclides included in the UK radioactive waste inventory. We do however recognise that small amounts of ^{233}U (that has a broadly comparable minimum critical mass to ^{239}Pu and also a significantly longer half-life of 160,000 years) are also contained within the inventory at disposal. Furthermore, ^{233}U will in-grow, in for example spent fuel over very long timescales, due to decay of ^{237}Np. However, ^{233}U has a much shorter half-life than ^{237}Np (2.14 million years) and thus decays before being generated in a mass sufficient to significantly affect spent fuel reactivity (see [73] for further discussion). Never the less, we have future work planned (see [10], task 132) which will further consider the potential for ^{233}U accumulations sufficient to achieve post-closure criticality and also seek to better understand the likely feedback coefficient of such an accumulation and therefore the type of transient event that they could hypothetically support.

Figure 23 Temperature feedback for ^{239}Pu oxide (PuO_2) for cylindrical systems in saturated NRVB at 40°C ambient temperature and 6.5 MPa ambient pressure. Figure produced from data presented in [70].



We recently assessed how criticality scenarios identified as credible (although unlikely) in a UK GDF may develop, and summarised relevant international research on transient criticality in the GDF [14]. Box 8 summarises the high level arguments as to why a post-closure rapid-transient criticality is not considered to be credible.

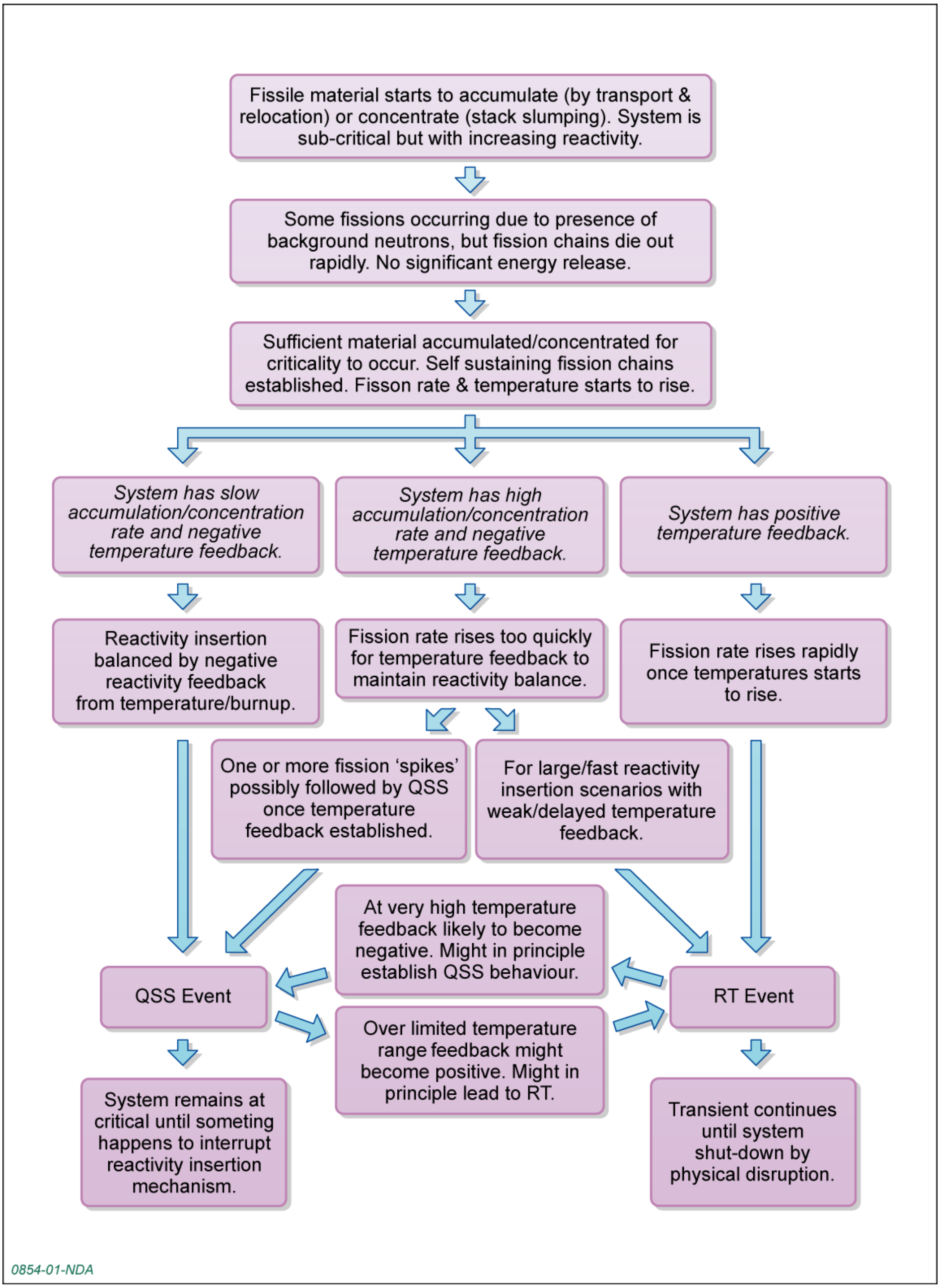
Box 8 Key feedback mechanisms that can affect the evolution of a critical system and the credibility of post-closure rapid transient criticality

Key arguments as to why a post-closure rapid transient criticality is not considered to be credible are:

- the timescale for credible critical systems to develop allows for substantial ^{239}Pu decay to ^{235}U (half-life of 24,100 years), meaning that any critical systems are likely to be primarily uranium-based.
- as the concentration of $^{239}PuO_2$ decreases and $^{235}UO_2$ increases, the probability of total positive temperature feedback for low concentration systems (typically <10 kg/m^3) decreases. By the time the system is almost entirely uranium-based, there are no systems with a low fissile concentration (in, for example, saturated bentonite) in which the total temperature feedback coefficient is positive. In particular, the Doppler-broadening feedback is substantially negative and would act more quickly than the water density component of the feedback. Therefore, if credible critical accumulations require at least 10^5 years to develop, then RT criticality at low oxide concentrations is not credible because the net temperature feedback will always be negative. Should such a system develop in a UK GDF, then the criticality would be a QSS transient.
- the only other parameter region in which any of the temperature feedback coefficients are positive (or are not conclusively negative when uncertainties are taken into account) relates to high fissile concentrations (above 500 kg/m^3). However, such concentrations assume that the fissile material almost completely fills any porosity in the host material, which would not occur in reality. Also, larger fissile concentrations require larger fissile masses (compared with the minimum critical mass for the configuration), so in order to develop such conditions the system may well have reached a critical QSS transient at an earlier stage. Furthermore, any (theoretically) positive Doppler-broadening feedback would be so small compared with the negative water density feedback, that even a partial contribution from a reduction in water density would be sufficient to ensure that any critical system could only develop as a QSS.
- internationally, a positive feedback mechanism driven by homogenisation rather than temperature has been conceived. However, no credible process has been identified that could provide the rapid homogenisation necessary to result in RT criticality in a UK GDF.
- RT critical systems are not considered credible in a saturated UK GDF; only QSS systems are (although unlikely), and only in the long term after closure of the GDF. RT criticality in partially-saturated GDF systems has not been assessed numerically as the UK GDF concept assumes saturated post-closure conditions (or dry conditions in terms of the evaporite concept).

In some cases, even if the reactivity decreases with temperature, there may be sufficient excess reactivity (for example, where there are sudden changes in the distribution of the fissile material) that the criticality behaves as a rapid transient rather than a quasi-steady state. The possible evolutions of a criticality are shown in Figure 24. The different types of criticality affect the potential release of radionuclides in different ways.

Figure 24 Schematic showing evolution of post-closure QSS and RT criticality events



In a QSS criticality the temperature in the neighbourhood of the critical region could be elevated for a considerable period (see subsection 6.2.2). This has the potential to modify processes locally in the disposal facility by modifying the chemistry, which may lead to enhanced corrosion rates, enhanced dissolution and release of gas, besides a greater mobility for radionuclides. The heat input may modify the groundwater flow through buoyancy effects and, coupled with chemistry effects, may modify the transport of the radionuclides. The higher temperatures in the neighbourhood of the critical zone could potentially lead to cracking (for example, of backfill or rock) as a result of thermal expansion. Finally, if a QSS operates for a long period during which there is continued accumulation of fissile material, it can lead to a modified inventory of radionuclides.

Note that Figure 24 only shows sequences leading to a criticality, and is not applicable in situations where a criticality does not occur. Even if fissile material starts to accumulate, a criticality could be highly unlikely; the branches do not represent equally likely outcomes.

In an RT criticality there could be locally (very) high temperatures for a very short period of time. This could provide a transient-enhanced release of radionuclides over the region affected by the criticality. The pressure generated by the criticality could lead to local deformation of the surroundings, including possibly the surrounding host rock. These deformations could open up existing cracks in the neighbourhood of the GDF and might create new fractures; it could also vitrify the surroundings. There is therefore a need to understand if these cracks could provide enhanced pathways for the groundwater and gas pathways to the biosphere. Finally an RT would be associated with radionuclide production (so the inventory would be increased). For a criticality event in the GDF these postulated events would occur deep underground.

6.1.1 Evidence from related criticality events

There is significant evidence (for example from natural analogues, criticality accidents and historical underground weapons testing programmes) to guide modelling and support the understanding that has been gained of hypothetical criticalities under GDF conditions.

Given the assumption, albeit very unlikely, that uranium and plutonium will separate from the other waste components and form critical masses moderated by water, the systems being assessed are in fact similar to some systems for which there are experimental results for critical systems. These include aqueous solutions and light-water moderated reactors. These systems provide data to validate the methods used to calculate the reactivity at low temperatures (less than ~350°C). Light water reactors also provide an example of negative thermal feedback leading to stable operation.

As noted in subsection 4.9, nature has provided us with one set of criticalities that occurred naturally deep underground – the Oklo natural reactors (see Box 4 in subsection 4.9). The high enrichment of the uranium (relative to present day values), the high concentrations of uranium, the lack of sufficient neutron absorbers, and the presence of sufficient water moderator were all pre-requisites for these natural reactors.

Based on a study of the residual uranium isotopes and fission products it has been estimated that the various Oklo reactors operated for between 200,000 and 800,000 years. The powers of the reactors were deduced to be of the order of several kilowatts per tonne of ^{235}U present. Operating temperatures have been deduced for some of the zones; these are in the range 180°C to 450°C. It was concluded that the reactors operated in a cyclic manner, probably as a result of water moving in and out of the fissile region.

The Oklo reactors demonstrate that 'just critical' conditions can be maintained over a long period of time. There has been successful modelling of some of the Oklo reactors on the assumption that the start-up of the reactors led to a burn-up of absorbers [35]. This increased the reactivity of the system, which was offset by the modest rise in temperature. Following burn-out of the absorbers, the accumulation of fission products, and the reduction in ^{235}U through fission, the criticalities eventually came to an end.

Some of the criticality accidents experienced during the development of the nuclear industry have resulted in a rapid transient of sufficient power to cause significant structural damage in the immediate vicinity [13]. To date these have been limited to two very similar uncontrolled critical excursions in research reactor facilities[33]. In each case a large amount of reactivity was inserted by a rapid withdrawal of a control or safety rod. In both cases the reactor fuel was highly enriched, so fuel temperature feedback was small. Termination of the fission chain was slightly delayed while heat was conducted into the water coolant, which has a large negative temperature feedback. By that time the fuel had melted and the criticality event was immediately followed by a large steam explosion.

Other, less destructive rapid transients have also been experienced in surface accidents, generally in systems containing solid fissile material [13]. In nearly every case the transient was terminated by some physical dispersal mechanism.

Compared with an event at the surface, a rapid transient underground will be much more highly contained, making dispersal more difficult but potentially leading to a higher release of energy.

6.2 Models for the consequences of criticality

We have developed various models that allow us to understand and bound the physical consequences of either extreme type of hypothetically possible criticality event taking place in the GDF during the post-closure period.

In subsection 6.2.1 we give an overview of our models that allow us to understand the consequences of post-closure criticality. In subsection 6.2.2, suites of calculations carried out under the UCuRC programme are described. Subsection 6.2.3 discusses how we have built confidence in one of our consequence models, by comparing it to the Oklo natural reactors (essentially benchmarking against a real underground criticality event). Finally, in subsection 6.2.4, our conservative bounding approach for estimating the consequences of a rapid transient criticality is presented.

6.2.1 Overview of model development

Models of how a post-closure criticality might initiate, progress and terminate may include reactivity effects, heat transfer, and the mechanical response of the surroundings. We have developed separate models for quasi-steady state and for rapid transient criticalities.

Although strong arguments and analysis (see Section 5) indicate that the likelihood of a post-closure criticality is low, it is considered prudent to extend and develop models for consequences of hypothetical criticality for use in the post-closure assessment. In fact, the environment agencies' guidance requires it [20]. If it can be shown that both the likelihood and the consequences (both the local physical consequences, and also the impact of such an event on post-closure GDF performance) are low, this is an example of multiple, parallel lines of reasoning that we can present in the safety case for the GDF (in the ESC).

The approach to model development has been to identify the key physics processes that are involved. These include reactivity effects, heat transfer, and the mechanical response of the surroundings (structural response). These can be treated at various levels of detail.

At one extreme it may be possible to demonstrate that the consequences of a criticality, for a given set of specified initial conditions, are minimal even when bounding assumptions are made. This is a robust approach to developing a safety case, provided the claim of 'bounding assumptions' can be supported.

[33] There was also a significant reactivity effect in the Chernobyl accident (which is not discussed in [13]), with a power surge leading to structural damage.

The approach that has been generally adopted is to develop models at an intermediate level of complexity, which are applied to simple conservative geometries, such as spheres and cylinders, as the ‘real’ geometry of any potential criticality is unknown. In some cases it can be argued that these simplifications are bounding. Because of the different key physics processes, and different timescales of the events, we have developed separate models for quasi-steady state transients and for rapid transients. These are the QSS and RTM codes, respectively. In addition, we have supported the further development of a more general multi-physics code, FETCH, which combines neutronics and thermal-hydraulics with some structural modelling. The main usage of FETCH is for rapid-transient modelling, where it can be compared with the conceptually simpler RTM code. More details of these codes are given in [30] and the references therein.

It is not directly possible to validate these models fully for GDF conditions. However, in many areas the models are based on well-established physics. For example, the RTM (and the simplified Bounding Approach that can also be applied) are based on the known phenomenology of underground explosions resulting from the detonation of chemical high explosives [28] and nuclear devices [29]. Furthermore, significant effort has been undertaken to ensure that the models are either already fit-for-purpose or that remaining gaps are identified, so that they can be addressed in the research programme. The main activities undertaken to provide confidence in the models are:

- peer review
- verification
- validation (in related areas, where there are data available)
- benchmarking
- sensitivity analyses.

These activities allow an assessment to be made of the uncertainties in the models’ predictions for a given scenario.

An independent peer review of the programme on Understanding Criticality under Repository Conditions was performed in 2006 [87]. The peer review, which included experts in neutronics and rock mechanics, focussed on the computational models that had been developed. The extensive and careful nature of the work was noted by the reviewers [87]. The difficulty in obtaining data for direct benchmarking was recognised, but further benchmarking against any existing data, such as Oklo (see subsection 6.1.1), was considered important. Given the lack of direct benchmarking information, the approach of developing two separate models for energetic transients (RTM and FETCH) was thought sensible, and the reasonable agreement between them was considered to give added confidence to the overall results.

Work on the validation, verification, benchmarking and uncertainty and sensitivity analysis of the three models is summarised in [30]. It is concluded that the computer models have generally undergone thorough verification (that is, checking that the computational models are consistent with the physical equations), both in terms of model construction and usage. This includes a number of checks to make sure that the results obtained are consistent with model assumptions and inputs, particularly for QSS and RTM. Benchmarking the computer codes is difficult, given that they aim to model regimes not typically covered by other models. Some benchmarking has been undertaken, such as comparisons between RTM and FETCH, which were developed independently, and opportunities do exist to undertake further benchmarks. These could assist in understanding the simplifications in the QSS and RTM, and the structural response models for RTM and FETCH.

Sensitivity studies have been fairly wide ranging for QSS and RTM, providing valuable insight into what may be the dominant uncertainties in the calculated results, and offering a route for the safety analyst to quantify uncertainty for stylised scenarios. These, in turn, could provide valuable insight for post-closure scenarios, when coupled to uncertainty for real or non-stylised models where geometrical variations and heterogeneity may be important. As a whole it is concluded that the uncertainties of the results are well understood where it is possible to make a judgement on likely variability, such as thermal conductivity or groundwater flow rate. For the more conceptual model inputs such as equations of state (the relationship between pressure, temperature and density) and structural response, judging variability is much more difficult. As a result, greater uncertainty will be present in RTM and FETCH results when compared to QSS results. For rapid transients, the use of bounding models is therefore a useful tool to provide upper bounds to uncertainty.

Some validation opportunities do exist, but no one experiment or natural scenario exists to fully validate any of the codes. However, the models can still be used with confidence, provided that they accurately reflect the physical processes, there is demonstrable verification, and account is taken of the key uncertainties in the application.

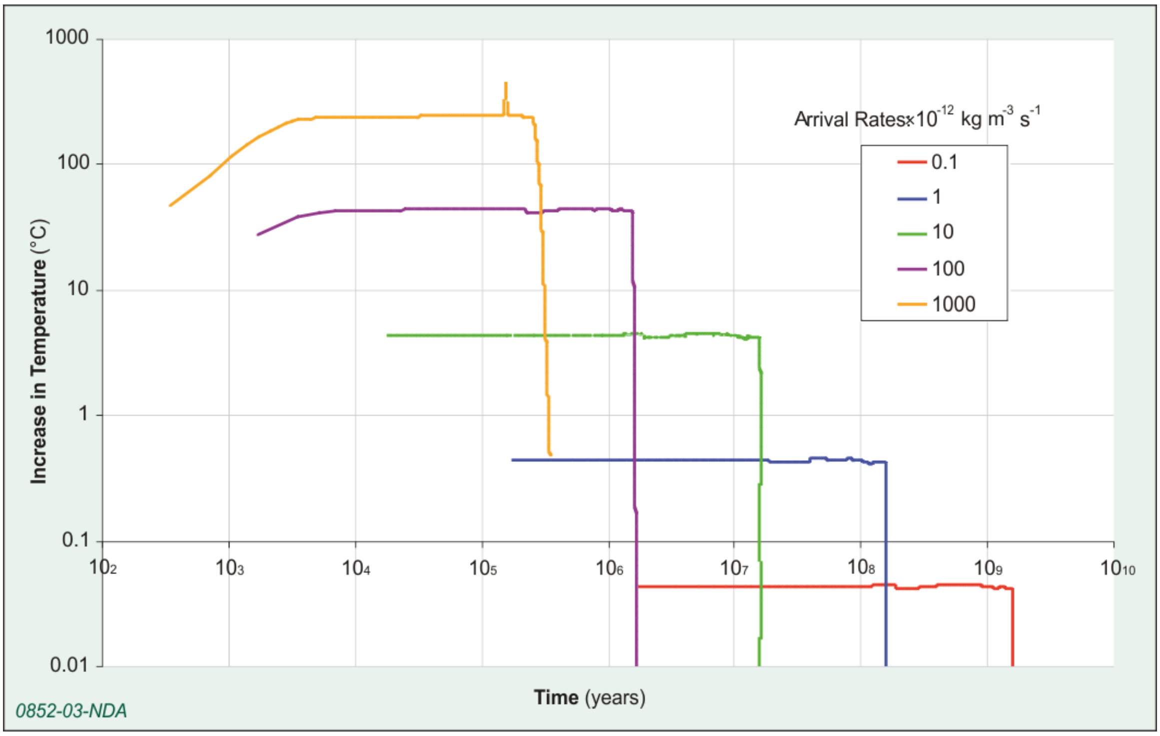
6.2.2 Suites of calculations

Having identified potential scenarios, a 'what-if' approach is taken to model calculations that often include extremes of parameter values, such as fissile mass. The calculations do not seek to reflect the likelihood of any scenario actually occurring.

The QSS and the RTM models were developed, and the FETCH code enhanced, so that the consequences of hypothetical post-closure criticalities could be assessed. Following an initial review of possible criticality scenarios, a set of calculations was specified for use in the assessment (see subsection 6.5). These calculations included extremes of parameter ranges, such as fissile mass, and so do not reflect the likelihood of any particular parameter or sequence. Thus, they provide a robust basis for assessing the range of consequences on the very cautious basis of a post-closure criticality occurring. The results of the calculations performed are provided in [88] and [89]. These calculations are largely for accumulations in backfill (NRVB) and granite (as a typical hard rock environment for an ILW concept). FETCH has also been applied to a number of scenarios, including stack slumping, and compared with the RTM results for a number of idealised scenarios, using simplified material properties.

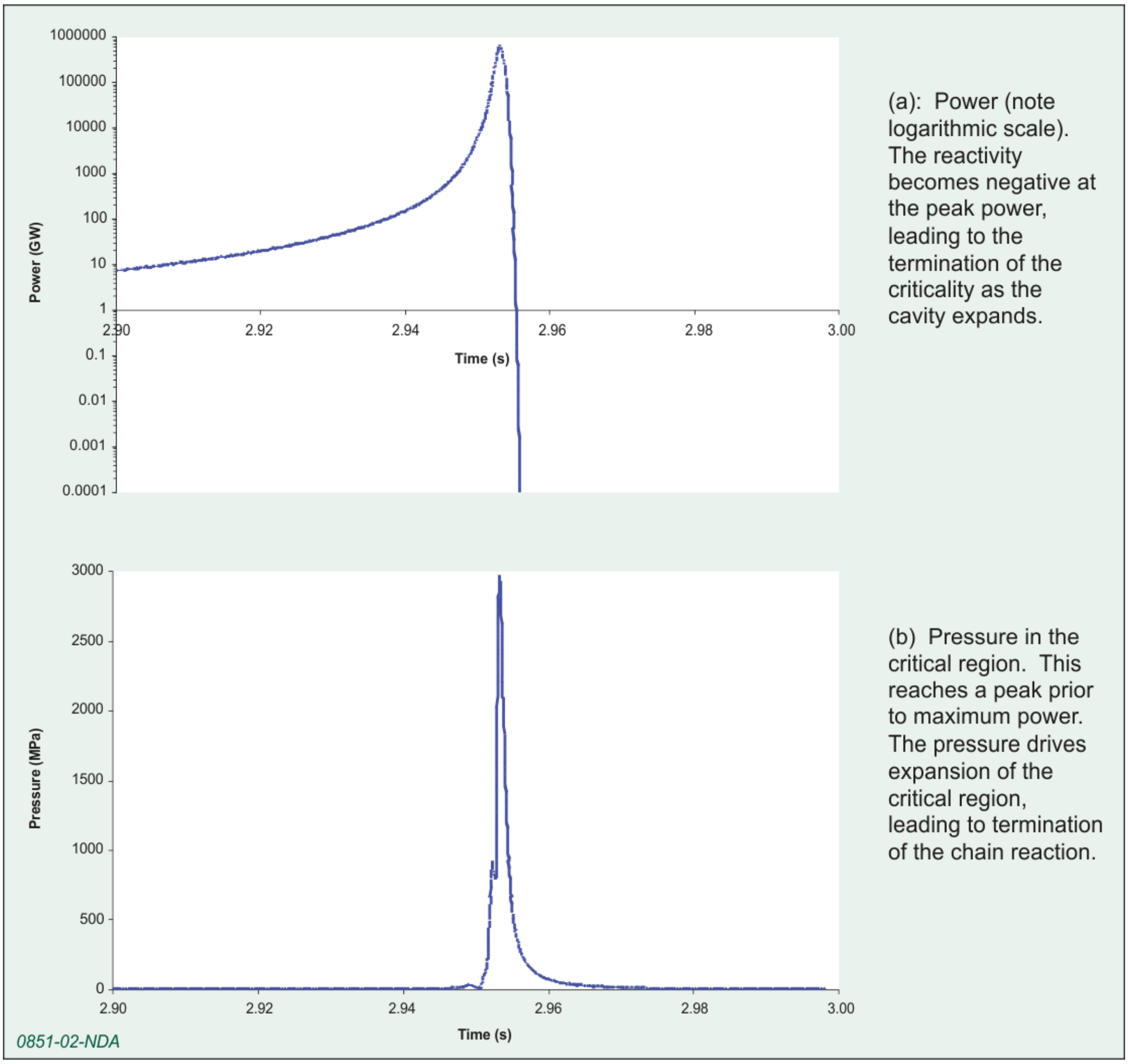
Information on using the QSS model and details about how it works are discussed in the consequences of criticality synthesis report [38] and our published QSS model user guide [90]. Example QSS calculations are shown in Figure 25 (from [88]). These are for a criticality of ^{235}U in NRVB, showing the effects of different accumulation rates; the assumption of pure ^{235}U is an example of the application of bounding, rather than realistic, scenarios. The results illustrate a common feature of the QSS calculations. Usually, after an initial transient, during which there is continued build-up of fissile material, the power, and thus the rise in temperature, are determined by the accumulation rate. It is seen that for low accumulation rates, which are consistent with the intention of low groundwater flow, the predicted temperature rise is small.

Figure 25 QSS transients for accumulation of ^{235}U in NRVB for a critical radius of 0.15m; the effect of different accumulation rates is shown [88]

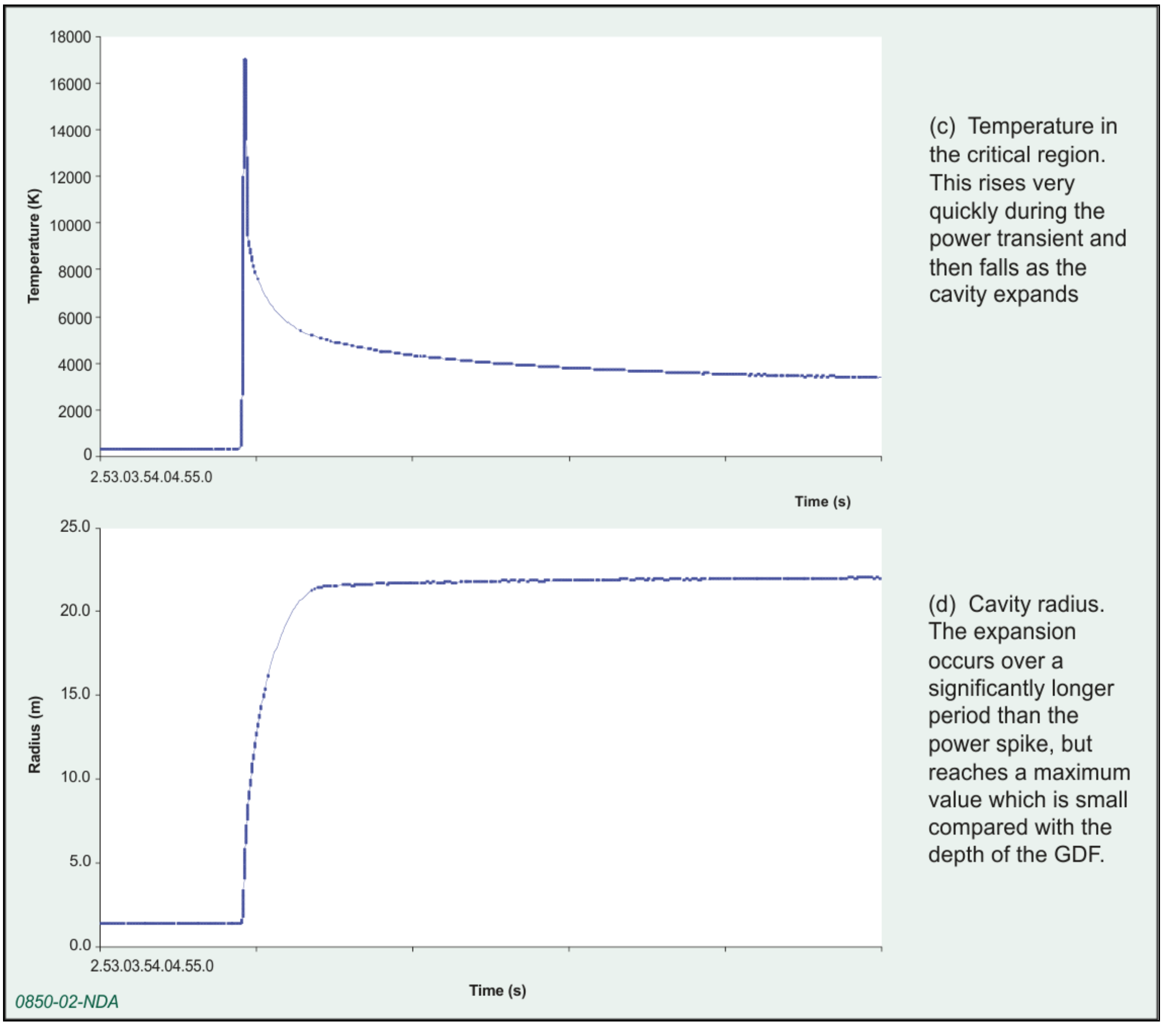


Information on using the RTM, along with a simplified Bounding Approach (see subsection 6.2.4), and details about how they work, are discussed in the consequences of criticality synthesis report [38] and our published Rapid Transient Model/Bounding Approach user guide [91]. An example of an RTM calculation for a rapid transient is given in Figure 26 [89]. Here the postulated criticality involves an accumulation of 100 kg of ^{239}Pu (this is an extreme accumulation example intended to illustrate RTM predictions; it should not be concluded that 100 kg is a realistic accumulation of plutonium oxide in the GDF). The calculations illustrate the rapid power rise associated with a rapid transient event, leading to high temperatures and pressures. The high pressure drives the expansion of the cavity on a timescale of the order of one second. This expansion terminates the criticality. In these calculations, it was assumed that expansion is into a region of backfill (NRVB). In practice, there will be greater resistance from the surrounding rocks, so the final cavity size is likely to be over-predicted in these calculations.

Figure 26 Criticality of 100 kg of $^{239}PuO_2$ (initial concentration 8.8 kg/m^3) in NRVB – RTM Calculations[34] (continued on following page). Figure produced from data presented in [89].



34 These calculations are intended to illustrate RTM predictions. It should not be concluded that 100 kg is a realistic accumulation of plutonium oxide.



(c) Temperature in the critical region. This rises very quickly during the power transient and then falls as the cavity expands

(d) Cavity radius. The expansion occurs over a significantly longer period than the power spike, but reaches a maximum value which is small compared with the depth of the GDF.

6.2.3 Modelling the Oklo natural reactors

We have built confidence in our quasi-steady state consequence model by benchmarking it against one of the Oklo natural reactors; a real, naturally occurring (~ 2 billion years ago) underground criticality event.

There is a good understanding of quasi-steady state criticalities. It has been possible, on the basis of the calculations performed, such as those in Figure 25, to deduce a ‘rule of thumb’ to scale results for different arrival rates; this is consistent with the understanding of the physical processes involved. The rule of thumb is summarised in Box 9.The main uncertainty in applying the model is the accumulation rate, which would be related to the groundwater flow and the solubility and sorption processes (including precipitation) for the fissile and other materials.

Box 9 The 'rule of thumb'

A key observation from sets of QSS criticality consequence calculations is the 'rule of thumb', which can be applied to scale consequence results for different fissile material or reactivity-insertion arrival rates.

This approach was first explained in [83] and can be summarised as:

- consider a system with a given arrival rate, which is not large enough for the system to reach temperatures where the pore water in the host material will boil (noting the boiling point of water at GDF hydrostatic pressure is significantly elevated above ambient, of the order of 200-300°C)
- suppose that at time t, while material is still arriving, this system has a temperature rise of ΔT above the ambient temperature
- also suppose that the power of the system is P, the neutron flux φ, and the composition of the fissile/fissionable materials is the vector C (concentrations of each radionuclide).

Now suppose that in a new calculation, the arrival rate of material is increased by a factor X. Provided X is not large enough for the system to reach boiling temperatures (or temperatures where positive temperature feedback is reached) the following will be approximately satisfied:

- at time t/X the temperature rise will be $X\Delta T$, the power XP and the neutron flux $X\varphi$, but the composition will still be C.

This general 'rule of thumb' can be applied over several orders of magnitude for X, and even applies to an extent if the system does undergo pore-water boiling.

As discussed in Box 4 (in subsection 4.9), the Oklo natural reactors demonstrate that 'just critical' conditions can be maintained over a long period of time. Box 4 also discusses how the availability of independent measurements, from which the conditions during the 'operation' of the natural reactors can be estimated, provides the opportunity to compare the natural reactors with results from the QSS model. We have therefore taken this opportunity to benchmark the QSS model against one of the Oklo reactors[35] [92]. Typically the reactor zones contained tonne quantities of fissile material.

Given the passage of about two billion years since the Oklo natural reactors operated, understanding the processes on the basis of measurements has limitations. There has been independent modelling of the reactor zone that has been the most studied (and as a result has the most data) by Naudet [35], on the assumption that the start-up of the reactors led to a burn-up of neutron absorbers. Our comparison studies therefore focussed on this reactor, zone 2. Using initial conditions for the QSS model consistent with those in [35], but using an independently formulated 'reactivity function' for the QSS model to represent the change in reactivity with temperature, uranium burn-up and the burn-up of neutron absorbers, a direct simulation of the zone 2 reactor was possible [92].

To establish whether the results of the QSS simulation are reasonable, data were required for a comparison. For Oklo zone 2 there are a number of independent measurements that can be used. From the concentrations and isotopic compositions of the residual fission products the burn-up can be deduced. The amount of fission allows the neutron fluence

[35] It is acknowledged that there were a number of reaction zones at Oklo, not all of which may have behaved in the same way. Alternative processes to those discussed within this report have been proposed in the literature. There is not currently a single consensus explaining the existence of the Oklo natural reactors.

(the total number of neutrons passing through a unit area during the criticality) to be estimated. Naudet [35] concluded that the fluence was about 8.7×10^{20} neutrons cm^{-2}.

The burn-up of ^{235}U can also be estimated from the measured uranium enrichment, which is less than that found in naturally occurring uranium. However, the difference is less than that required to explain the estimated burn-up based on the fission product measurements. The reason is that ^{239}Pu is created by neutron capture in ^{238}U. Some of the ^{239}Pu would have undergone fission itself, but some would have decayed to form ^{235}U. The ratio of fission to decay of ^{239}Pu depends on the power and duration of the reactor. This enabled deduction by Naudet that a reactor lifetime of about 620,000 years is consistent with the measured uranium enrichment. The analysis also allows the burn-up of uranium, which is the fraction of uranium mass (both ^{235}U and ^{238}U) that has been converted to other radionuclides through fission and capture, to be estimated; giving an average of 0.7% over the reactor.

The presence of uranium oxide in the form of uraninite indicates an operating temperature in the range 300-350ºC. The ambient temperature at the depth at which the zone 2 reactor is believed to have operated is 160ºC. It is concluded that the temperature rise produced by the zone 2 reactor was about 140ºC.

The above values, deduced independently from measurements, are a sufficient set to undertake a meaningful comparison with a QSS simulation of the Oklo zone 2 reactor.

Table 4 shows a comparison of the QSS results with each of the estimates from the measurements discussed above. No parameters were tuned in the QSS model to attempt a 'fit' to any of the measured values. Table 4 shows good agreement between the measured data and the results from the QSS model simulation, with the agreement being within a factor of two for each of the quantities compared.

Table 4 Comparison of estimated (Naudet [35]) and calculated (QSS) values for Oklo zone 2. Data reproduced from [92,93].

Parameter	Units	Estimated	QSS
Duration	years	620,000	500,000
Burn-up of uranium	%	0.7	0.9
Fluence	neutrons cm^{-2}	~8.7 10^{20}	4.5 10^{20}
Temperature rise	ºC	~140	100

The successful comparison of the QSS model with one of the Oklo natural reactors builds confidence in our modelling approach for quasi-steady-state criticality events. This example of how we seek to benchmark and compare our approach with available information has been communicated internationally through a criticality conference [93], and a peer-reviewed published journal article [37].

6.2.4 A bounding approach for a rapid transient criticality

In our rapid transient model there is a significant coupling between the neutronics and the rock structural response. Because results are subject to significant uncertainty we have developed a simpler, conservative bounding approach to calculating the consequences of a rapid transient criticality.

There is significant coupling between the neutronics and the structural response modelling for rapid transients. The nuclear data for the neutronics modelling are generally well-established, even for very high temperature systems. However, there are still significant uncertainties in the structural response modelling. Nonetheless, there is a good experimental database [94] relating cavity size to the energy release. In the rapid transient events, the early growth of the cavity is likely to be important in restricting the energy release. This is difficult to model, because of the need to develop equations of state that apply at high temperatures and pressures to the material in the criticality, and because of the transient loading on the surrounding rock.

Following a detailed summary of the status of the transient criticality models (including verification, validation, benchmarking, uncertainty and sensitivity analysis) [30], it was concluded that the results of RTM calculations were subject to significant uncertainty associated with supplying realistic parameters for the equation of state and structural response parameters to the model.

A simpler Bounding Approach model was therefore proposed to conservatively demonstrate that a rapid transient has limited consequences, and the idea was subsequently developed and applied to a range of hypothetical RT criticality events under the scenario of accumulation [94]. It is a simplified version of the RTM and involves bounding the energy release by assuming that there is no expansion. In this case, the material will reach a temperature at which the criticality has terminated. Having obtained the energy input by this route, the consequences on the surroundings can be evaluated using pessimistic empirical data; hence empirical relationships are used to estimate the radius of the cavity that could form, and the extent of cracking to the host material [94]. It then remains to show that a sub-critical state will be maintained by the expanded fissile region on cooling.

The Bounding Approach typically gives energy releases a factor of three to four higher than those obtained when modelling the transient with the RTM [30]. A factor of four in energy corresponds to an increase of 60% in the cavity radius. The Bounding Approach model will, therefore, bound the energy release compared with an RTM calculation for the same hypothetical criticality event, although the consequences in terms of cavity radius are not unreasonably over-estimated.

6.3 Further assessment of the consequences of criticality

More recent research has considered consequences of criticality for a broader range of types of waste (ILW, LLW, DNLEU, HLW, spent fuel, plutonium and HEU) in higher strength rock, lower strength sedimentary rock and evaporite.

For static criticality analysis, work conducted by RWM between 2011 and 2014 has served to:

- gain a more detailed understanding of the conditions that would have to develop for post-closure criticality in different 'what-if' scenarios
- quantify the effects of the radioactive decay of plutonium (where applicable) on critical configuration, and the associated impact on the possibility of rapid transient criticality events.

For transient criticality analysis the work of RWM:

- applied the QSS and Bounding Approach models to scope the consequences of a sufficient range of criticality transients.

The programme considered three general 'what-if' scenarios, as described in Section 4 (in-package, single package and multiple package accumulations). Table 5 shows how the generic scenarios are applicable to the different waste types for geological disposal; HLW does not pose a criticality risk for any of the identified scenarios.

Table 5 Summary of which 'what-if' scenarios apply to which waste types

'What-if' scenario	ILW, LLW or DNLEU	HLW	Spent Fuel	HEU	Plutonium
Accumulation	Yes	*	Yes	Yes	Yes
Stack slumping	Yes	N/A	N/A	N/A	N/A
In-package	†	*	Yes	Yes	Yes

Notes:

* Although theoretically applicable, the low fissile content of HLW means that in-package criticality is not possible. Furthermore, the contents of multiple high-integrity packages would need to relocate for the accumulation scenario, which is not considered credible.

† For the small number of ILW and DNLEU (the LEU component) packages that contain sufficient fissile material for in-package criticality, it is considered that the accumulation scenario (accumulation in the encapsulant grout) can be considered instead of specific in-package analysis, because significant rearrangement/relocation of material within the package would be required for a critical configuration to be credible.

The analysis for the 'what-if' scenarios, as applied to different waste types and different illustrative disposal concepts is summarised in [38], which is underpinned by two detailed technical reports [76, 95]. The key conclusions of this work, which underpin our understanding of post-closure criticality safety, are described below.

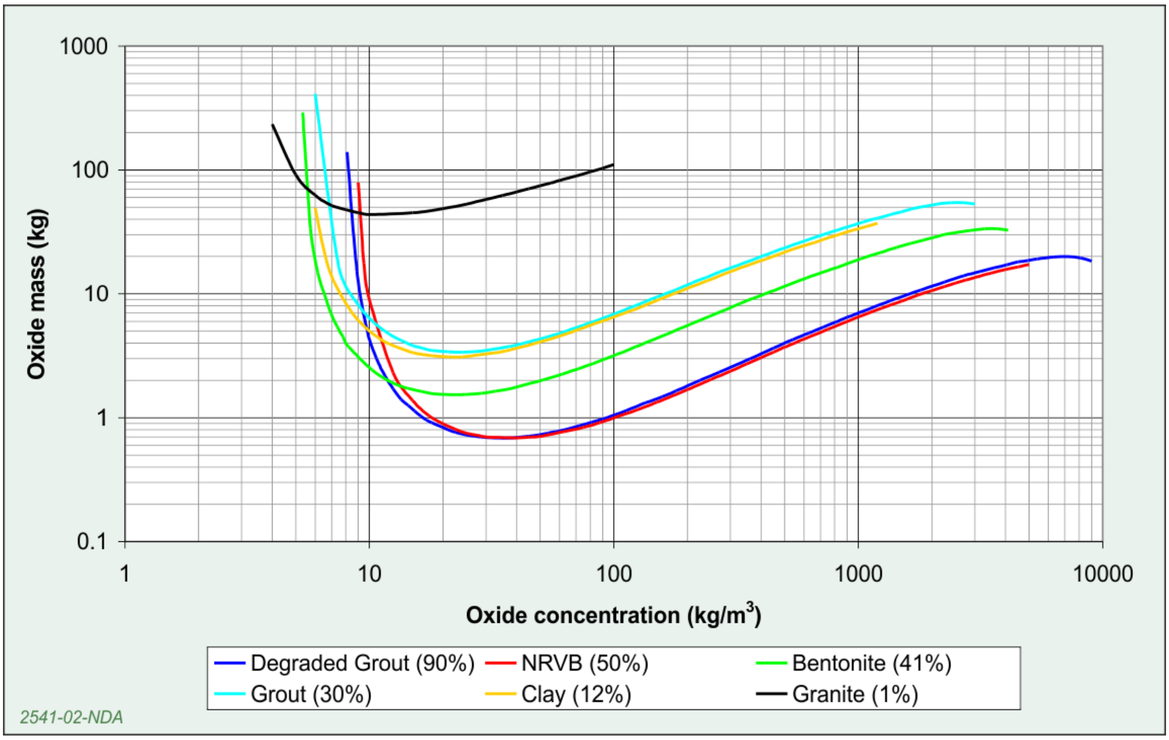
6.3.1 The accumulation scenario

Rapid transient criticality is only possible over a narrow range of ^{239}Pu concentrations; due to decay this becomes less likely the longer the accumulation takes. If it did happen, a cavity of a few metres and host rock cracking of tens of metres could occur. For a quasi-steady state criticality, the power would be less than a few kilowatts and the extent to which the temperature rise is above 10°C is a few metres.

The 'what-if' accumulation scenario applies generally for geological disposal, and was the basis for the development of the transient criticality software models during the UCuRC programme. Assuming the transport of fissile materials from one or more waste packages, and some mechanism for deposition in a localised region of the GDF, the accumulation could occur within encapsulant materials, backfill or buffer materials, or the host rock. Assuming that accumulation occurs within an idealised sphere, static criticality calculations for accumulation in a range of materials have shown that critical masses are hypothetically possible in the waste encapsulant (grout), NRVB, bentonite, granite (higher strength rock), and clay (lower strength sedimentary rock). No critical configurations were found for accumulation in evaporite rock since the evaporite specification used had a low porosity and a chemical composition including chlorine, which is an effective absorber of neutrons. Should a different evaporite composition or higher porosity be considered then a critical configuration could be possible.

Figure 27 shows the conditions that would be necessary for critical configurations of ^{239}Pu (as an oxide) from accumulation in a number of different host materials. The assumed porosity for each material is given alongside the material name in parentheses. The figure shows that porosity is a key control on the critical configurations, but is not the only factor affecting this. Had porosity been the only control, then the curve for clay (12% porosity) would have been between that for granite (1%) and grout (30%), for example. In each curve in Figure 27 there is a minimum critical mass, below which criticality is not possible. It is seen that this varies considerably over the range of host materials, from about 0.7 kg in NRVB or highly degraded grout, to about 3 kg in clay or over 40 kg in granite.

Figure 27 Comparison of critical masses for the accumulation of ^{239}Pu (oxide) in a range of host materials [38]



The curves in Figure 27 generally represent the minimum conditions for criticality within a given material as a function of the concentration of fissile material. If the fissile material is ^{235}U, or possesses a lower enrichment of uranium then the masses required for criticality are larger. This is shown in Figure 28, which compares the critical masses for accumulation in bentonite for combinations of plutonium and uranium.

In Figure 28, the curves for different ratios of Pu:U are representative of zero, one, two, four and infinite half-lives of ^{239}Pu. For example, 50:50 Pu:U is 50% ^{239}Pu and 50% ^{235}U. Different levels of enriched uranium are also shown, for example, 100U10 is 10% enriched uranium. After 7 half-lives any ^{239}Pu originally present would be less than 1% of the remaining fissile material. Some important trends are observed. Firstly, as ^{239}Pu decays to ^{235}U, the minimum mass for criticality increases. Secondly, if neutron absorbers such as ^{238}U are present, then the minimum mass for criticality increases further; for example, the minimum mass for the ^{235}U system is about 2.5 kg [95]. This increases to 627 kg of uranium when enriched at 3%, which corresponds to 18.8 kg of ^{235}U [91].

The black diamonds in Figure 28 are significant in understanding the effects of ^{239}Pu decay. In a similar way to Figure 23, these points show the transition from positive temperature feedback at low concentrations to negative temperature feedback at larger concentrations.

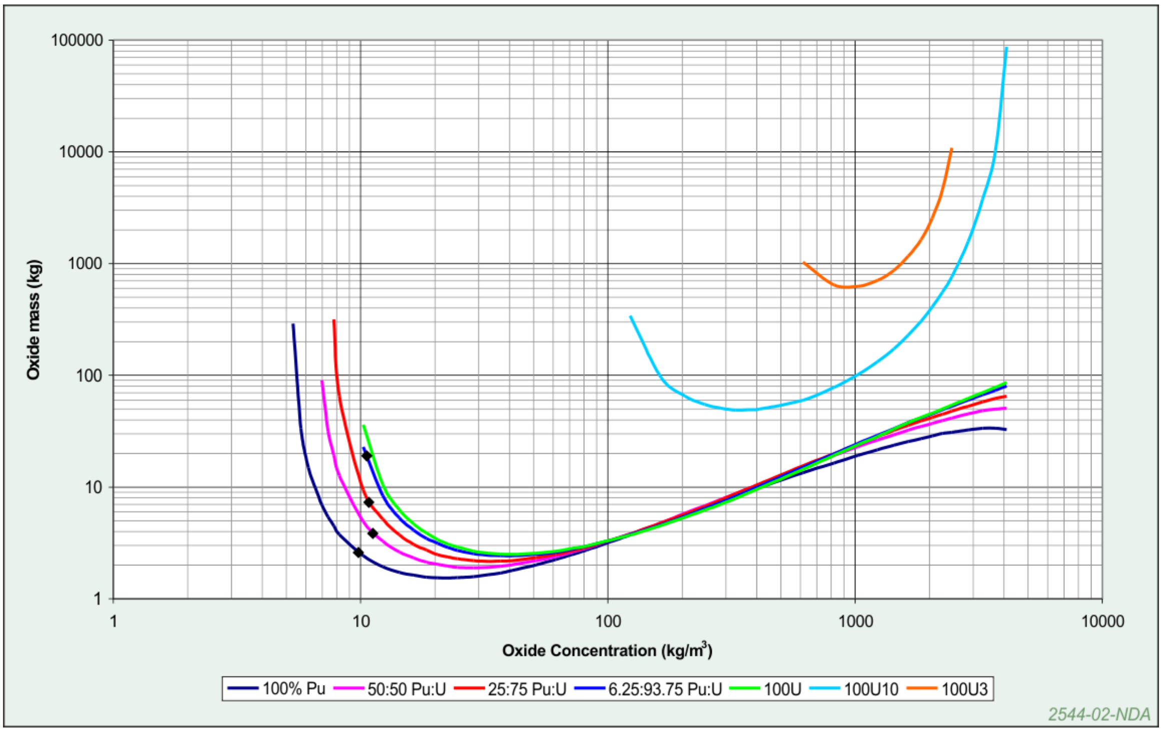
Curves with no marker only have negative temperature feedback. Three significant observations are made.

- for ^{235}U, no systems with positive temperature feedback are found, so that rapid transient criticality would not be possible
- the fissile concentration range over which the temperature feedback is positive is narrow, from about 5 kg/m^3 to 10 kg/m^3, and this range becomes narrower as ^{239}Pu decays to ^{235}U
- the minimum fissile mass for positive temperature feedback increases significantly as ^{239}Pu decays, from about 2.6 kg for a ^{239}Pu system to about 20 kg after four half-lives of radioactive decay.

The combination of the above trends suggest that the longer it takes for a hypothetical critical accumulation of ^{239}Pu to occur, the less credible a rapid transient criticality becomes, with the expectation that rapid transient criticality is not credible for hypothetical critical accumulations that require post-closure timescales in excess of 100,000 years to develop.

The observations are not specific to accumulation in bentonite and similar trends are observed in different potential host materials. For accumulation in granite it was also shown (from static calculations) that no critical configurations were found with the fissile material as either 10% enriched or 3% enriched uranium (indicating that neither QSS or RT criticality were possible).

Figure 28 Critical masses of plutonium and uranium (oxide) accumulation in bentonite (porosity 41%), with estimates (black diamonds) of where the switch from positive to negative temperature feedback occurs as the fissile concentration increases [38,95]



The UCuRC programme undertook a range of transient criticality calculations for different accumulations of fissile material in NRVB. Under the Modelling of Consequences of Hypothetical Criticality programme the analysis was extended to grout, degraded grout and bentonite systems [38]. It is noted from Figure 28 that since the majority of critical systems have negative temperature feedback then most hypothetical criticality events would evolve as quasi-steady-state systems, if maintained by the continued accumulation of fissile materials.

Bounding approach calculations

To scope the consequences of rapid transient criticality events from accumulation, the Bounding Approach was used. Most of the calculations considered the accumulation of 10 kg of fissile material. A smaller number used a larger mass of 100 kg. This is not because 100 kg is considered a credible accumulation mass, but for comparison with earlier calculations from the UCuRC programme, and to show that even if we hypothesised extreme criticality events the local consequences to the GDF are still not significant (that is, the GDF could tolerate them).

For the calculations assuming 10 kg of fissile material the energy releases are limited to less than 125 GJ [95]. The equation that relates energy to cavity radius is summarised in Box 10.

Box 10 The relationship between energy release and cavity radius

For Bounding Approach calculations the key result of interest is the energy release in Joules[36]. From the energy release an estimate of the cavity radius formed by the energy release can be calculated from the empirical relationship [94]:

$$R_c \approx c\left(\frac{W}{4.18\times10^{12}}\right)^{1/3}$$

where R_c is the cavity radius (the radius that vaporises following an energetic release) in metres, W the energy release in Joules, and c is an empirical coefficient, dependent on material type and with units m $kt^{-1/3}$. This relationship was established from underground explosive tests, although it also has a sound physical basis in that taking the cube of the equation, the relationship is essentially that the vaporised volume is proportional to the energy release. The coefficient c is a (dimensional) number of the order of 10 although this varies between different materials, with quoted values of 7.6 m $kt^{-1/3}$ for dense carbonate rocks (such as dolomite or limestone) and 11 m $kt^{-1/3}$ for dense silicate rocks (such as granite).

For NRVB, as a ‘soft’ material, it was proposed in [94] that the value could be as large as 20 m $kt^{-1/3}$ since NRVB is weaker and less dense than carbonate or silicate rocks. With these representative values it is useful to apply each of these factors to the energy release to understand the range of cavity radii that could result from a hypothetical rapid transient event.

Further length scales of interest are the radii to which cracking may occur. Using data from conventional and nuclear underground tests, the general view [94] is that there is:

- a high permeability (crushed) region of about 2 to 3 R_c
- a fracture / shear failure zone region of about 4 to 5 R_c
- a radial cracking region of about 10 to 14 R_c, although it is noted that beyond about 3 R_c there is very little change to the permeability of the rocks, even though some fracturing and cracking may have occurred.

The radii of these regions can therefore be estimated from the cavity radius for each calculation.

Assuming a bounding estimate of the cavity radius, the maximum estimate is the formation of a cavity of radius 6.2m, and hence the extent of cracking would be of the order of tens of metres at most [95]. Another important observation is that for equivalent initial fissile masses in the same material, an increasing fraction of ^{235}U always reduces the energy release, and generally in ratio to the proportion of ^{239}Pu. For example, if the energy release for 10 kg of ^{239}Pu is 100 GJ, then for 10 kg of ^{239}Pu:^{235}U in ratio 25:75 (representing two half-lives of decay) the energy would be approximately quartered [95]. Box 11 explains why this is the case, that is to say, what it is about criticality from plutonium systems that makes the consequences greater.

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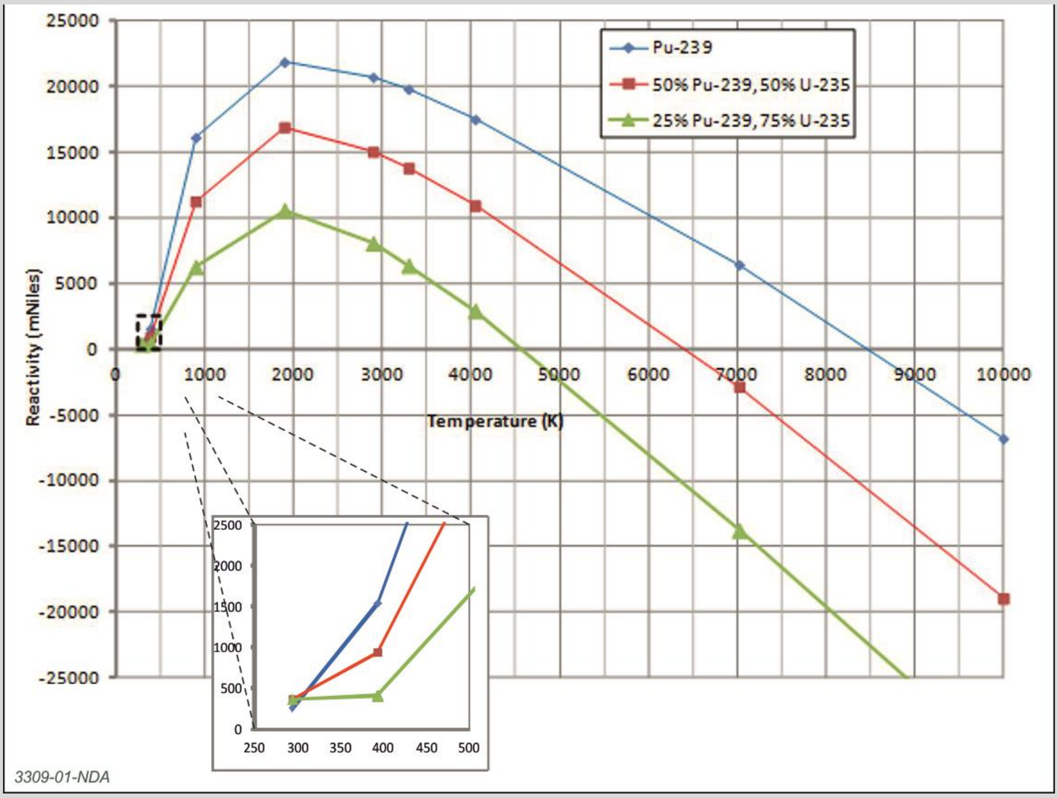
36 Energy values are also sometimes given in kilotons (kt) of TNT equivalent.

Box 11 Why Pu criticality events yield greater physical consequences

The consequences of hypothetical rapid transient criticality events from equivalent initial fissile masses in the same host material depends on the ratio of plutonium to uranium – the higher the plutonium content the larger the local consequences. This is due to the magnitude of the positive Doppler broadening feedback coefficient (also referred to as the nuclear data feedback), which is the key component of the temperature feedback for such hypothetical systems. As ^{239}Pu decays to ^{235}U the magnitude of the Doppler broadening feedback weakens. Generally, for initial temperatures consistent with GDF conditions the ^{239}Pu feedback is positive and the ^{235}U feedback is negative, so that as the fraction of ^{235}U increases (from radioactive decay) the weaker this feedback becomes. At a sufficiently high ^{235}U fraction the feedback becomes negative and a rapid transient system cannot occur.

The effects of Doppler broadening can be further illustrated by considering how the reactivity of a hypothetical critical configuration varies as a function of temperature, as used for the Bounding Approach model. The figure below gives an example of static fissile accumulation calculations in 75% porous grout.



Firstly, it can be seen (most readily in the inset part of the figure) that as the fraction of ^{235}U increases so the initial slope (the Doppler feedback coefficient) reduces, and that the initial slope would become negative for a sufficiently large ^{235}U content. Where the initial feedback is positive, the energy release from that system is closely related to the integral of the reactivity over the temperature range where the reactivity is positive (strictly where the reactivity exceeds prompt criticality). It can be deduced that the area under the curve for the 50:50 mix is about half that for 100% ^{239}Pu, and for a 25:75 mix it is about halved again.

The Bounding Approach calculations also provide an understanding of the effects of the accumulated mass on the consequences of criticality. A comparison of calculations with 10 kg and 100 kg of ^{239}Pu shows that the consequences of the criticality events (the cavity radius and radius of cracking) are about three times larger for a factor of ten increase in mass. This is because the increase in mass from 10 kg to 100 kg increases the energy release by a factor of about forty, and since the cavity radius and radius of cracking scale with the cube root of the energy release the local consequences increase by a factor of about three. If the decay of ^{239}Pu is taken into account (that is, a larger mass requires longer to accumulate and hence there would be more radioactive decay), then the consequences would reduce.

QSS calculations

QSS calculations for accumulation in grout, degraded grout and bentonite have shown similar trends to those observed during the UCuRC programme, including following the 'rule of thumb' (see subsection 6.2.3 and Figure 25). It is generally observed that for all of the different accumulation systems considered, including those from the UCuRC programme, then for mass accumulation rates of up to the order of 1 g/year:

- the temperature rise of the fissile material region is generally lower than that required to boil the pore water
- the power of the transient criticality is less than a few kilowatts
- the spacial extent to which the temperature rise surrounding the critical volume is above 10°C is a few metres.

Larger temperature rises and power are only predicted for larger arrival rates of the fissile material, which typically require the pore water in the fissile material region to boil. However, porewater boiling will generally act to not only prevent accumulation of fissile material, but also acts to reduce neutron moderation, and therefore to cease the excursion[37].

Another significant observation of the QSS calculations is that, for comparable arrival rates, the local consequences from QSS calculations are larger for a system initiated from ^{239}Pu accumulation compared to ^{235}U accumulation. This is a typical trend for QSS calculations for different host materials.

For calculations with the QSS model, the general approach (from the UCuRC programme and subsequently) was to consider a range of arrival rates for a given initial condition, and hence to establish trends with this model input. Following work from the Likelihood of Criticality programme further quantification of arrival rates has been possible. Using specific examples from the Likelihood of Criticality programme [72, 73], arrival rates between about 10^{-14} and 10^{-8} kg/m^3/s have been estimated [38, 76]. These rates are broadly similar to those used in the analysis of the consequences of hypothetical QSS criticality events.

[37] At a pressure of 6.5 MPa (corresponding to an assumed depth of 650 m) pore water will boil at about 280 °C. If the fissile material region exceeds this temperature then the evaporating water (requiring more volume as steam) will act to displace surrounding water away from the fissile region, and being a long duration event, there will be time for this to occur. In doing so, the capacity for further fissile material to accumulate will be reduced, or even stopped, since the assumption is that there is some underlying flow of groundwater to transport fissile materials.

6.3.2 The stack slumping scenario

Critical configurations (both QSS and RT) are only possible if the encapsulant grout is sufficiently degraded and there are kilogram quantities of fissile radionuclides that can slump together. A rapid transient criticality event from stack slumping scenarios (assuming 7 kg of fissile material) would release energy limited to the order of tens of gigajoules. Quasi-steady state events (for a wide range of slumping rates) are calculated to produce power limited to a kilowatt, and a localised temperature rise (of the critical region) of up to 170°C.

The stack slumping scenario, where it is assumed that fissile materials can slump with gravity through a stack of degraded waste packages, can only be hypothesised for ILW, LLW and DNLEU disposal in the illustrative disposal concepts, as these are the only waste packages that are stacked. The scenario was not modelled with the QSS model, RTM or Bounding Approach model during the UCuRC programme[38]. During the Modelling of Consequences of Hypothetical Critical programme, the QSS model was extended to enable its application to the stack slumping scenario.

For a conceptual model of a stack of seven waste packages with a radius of 0.4m and an initial height of 8.7 m, analysis was undertaken to determine the conditions required for criticality [76]. The studies included different fissile masses and different porosity values for the grout encapsulant (an increase in porosity representing degradation of the grout). A range of slumping factors (rates) was considered [76]. As an example, a slumping factor of 0.8 would mean that the upper 80% of the fissile material has slumped into the lower regions of the stack (that is, all of the fissile material has relocated into the lower 20% of the original stack height) with a fissile region height of 1.74 m, and hence a cylindrical fissile region with a height just over twice its diameter [76].

Individual package fissile contents of 250 g, 500 g and 1 kg were considered, giving total masses for a stack of seven drums of 1.75 kg, 3.5 kg and 7 kg. Both ^{239}Pu and ^{235}U systems (as oxide) were considered [76]. The selection of these cases for investigation was for illustrative purposes only. In particular, it is recognised from [72] that significant degradation of grout is expected to take at least of the order of 100,000 years. Given the half-life of ^{239}Pu, any hypothetical slumped system is therefore expected to contain low levels of ^{239}Pu, making an RT event from stack collapse vanishingly unlikely. However, from the viewpoint of scoping the consequences of hypothetical criticality events, the consideration of ‘worst cases’ such as ^{239}Pu slumping can be considered to bound the consequences of hypothetical criticality.

Figure 29 shows the results of criticality calculations for a range of porosities of the degraded grout and a range of slumping factors for the slumping of 7 kg of ^{239}Pu. $K_{effective}$ is shown as a function of how far the fissile material has slumped. The region of interest is where $K_{effective}$ is greater than or equal to unity, representing critical or super-critical configurations. Of particular interest is the slumping factor where $K_{effective}$ first equals unity, since this would represent the onset of a transient criticality event from stack slumping. Figure 29 shows that for 7 kg of ^{239}Pu, the slumping factor needs to be between about 0.82 and 0.85 (dependent on porosity) for a critical configuration to be established. At very high slumping factors the fissile material becomes so concentrated that moderation is limited and the system becomes sub-critical.

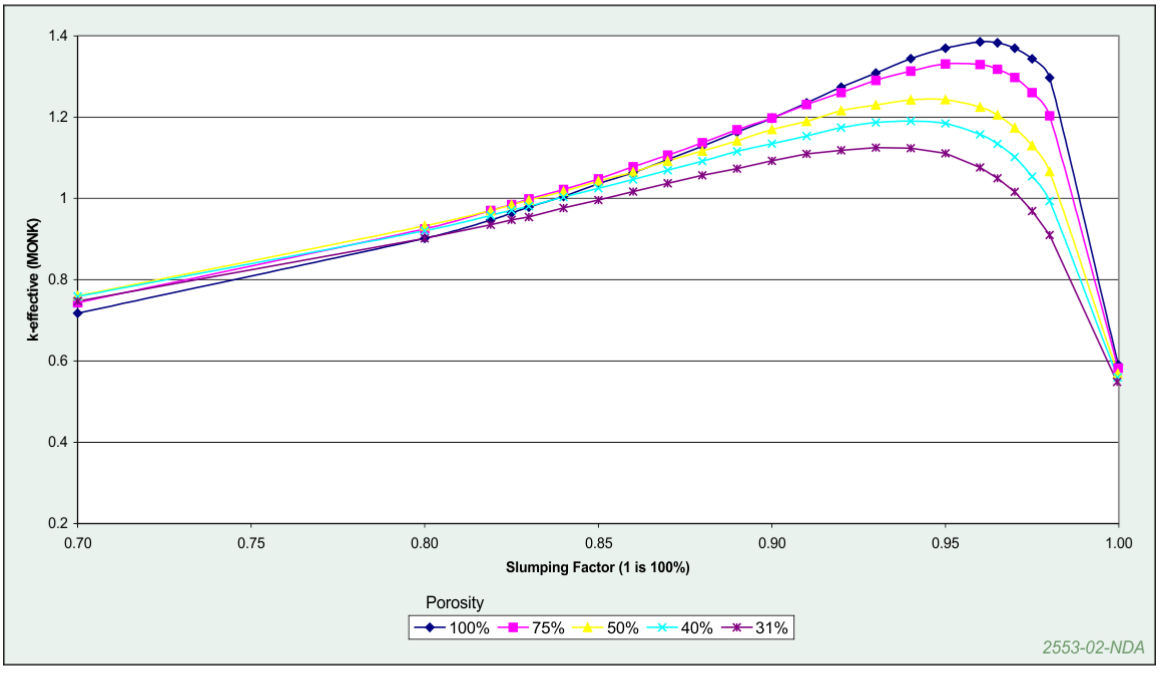
For a lower mass of fissile material within the stack of packages, a greater slumping factor is required for a critical configuration. For example, if there were a total of 3.5 kg of ^{239}Pu, the slumping factor needs to be about 0.92 for a critical configuration. For 1.75 kg of ^{239}Pu it would not be possible to reach a critical configuration, irrespective of the slumping factor

[38] Stack slumping was modelled in the UCuRC programme using FETCH.

and porosity of the grout (this observation is broadly consistent with the single package plutonium screening levels discussed in subsection 3.4). For a ^{235}U system the slumping factor would need to be greater than for the same fissile mass in a ^{239}Pu system.

Calculations of temperature feedback coefficients for hypothetical critical configurations following slumping show that (as for the accumulation scenario), positive temperature feedback (and hence rapid transient criticality) can only be found if sufficient ^{239}Pu is present.

Figure 29 Summary of MONK calculations for the slumping of 7 kg of ^{239}Pu (oxide) in grout of varying porosity [76]



Analysis of hypothetical criticality events for the stack slumping scenario included use of the Bounding Approach model for hypothetical rapid transient criticality events, and the QSS model for quasi-steady-state criticality events. The results are discussed below.

Bounding approach calculations

The results from Bounding Approach calculations from stack slumping (each assuming 7 kg of fissile material) are consistent with those from the accumulation scenario, where for fissile masses of up to 10 kg, the energy release is limited to the order of tens of gigajoules, equating to a cavity radius of less than 4.3 m [76]. It was also observed that the decay of ^{239}Pu to ^{235}U lowers the energy release.

QSS calculations

QSS calculations were undertaken [76] for slumping of 7 kg of ^{235}U at different rates of slumping (the rate at which the height of fissile material in the slumped waste stack reduces). In the calculations the initial height was 0.811 m. This means that the fissile material from seven waste packages would have to slump into less than 10% of the original stack height. The calculations end when the height is 0.16 m (20% of the original height), so the duration of slumping at a rate of 10^{-11} m/s is about 2,060 years. At a slumping rate of 10^{-14} m/s, the duration is over 2 million years. Given that significant degradation of grout is expected to take at least of the order of 100,000 years [34], and slumping occurs over length scales of several metres, slumping rates of the order of 10^{-12} m/s, or lower are considered the most realistic. It should however be noted that additional scenarios can be envisaged that could result in quicker slumping rates; for example, seismic activity triggering sudden slumping of a heavily degraded grout system.

The temperature and power predicted from QSS calculations are shown in Figure 30 and Figure 31. The results are similar to those for accumulation calculations (that is, similar temperature rises have similar power). In general, Figure 30 and Figure 31 show that the behaviour of the stack slumping calculations follows similar behaviour to the QSS accumulation calculations where the arrival rate is replaced by the slumping rate, provided this rate is sufficiently small. At the largest slumping rate of 10^{-11} m/s the behaviour is different. In this case, the temperature plateaus at just over 210°C (a temperature rise above ambient of about 170°C). The power also plateaus at about 1000 W. The explanation for this is that were the pore water to boil, no critical configurations would be possible. Since a quasi-steady-state criticality requires a continued just-critical configuration; the temperature will therefore be limited to values below the boiling temperature of water at GDF depth/pressure.

Figure 30 Average temperature increase of the fissile material region as a function of time for stack slumping of 7 kg of ^{235}U in 75% porous grout. 1 pm/s = 10^{-12} m/s for the slumping rates [76].

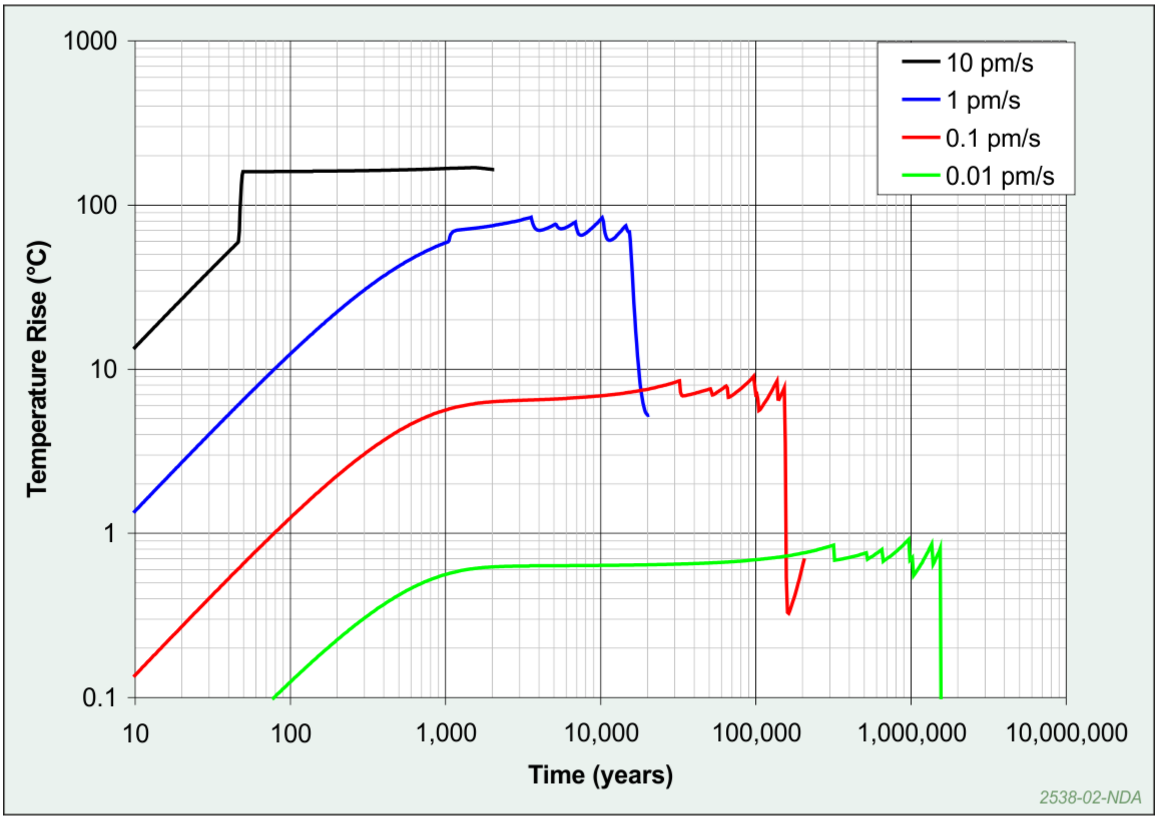
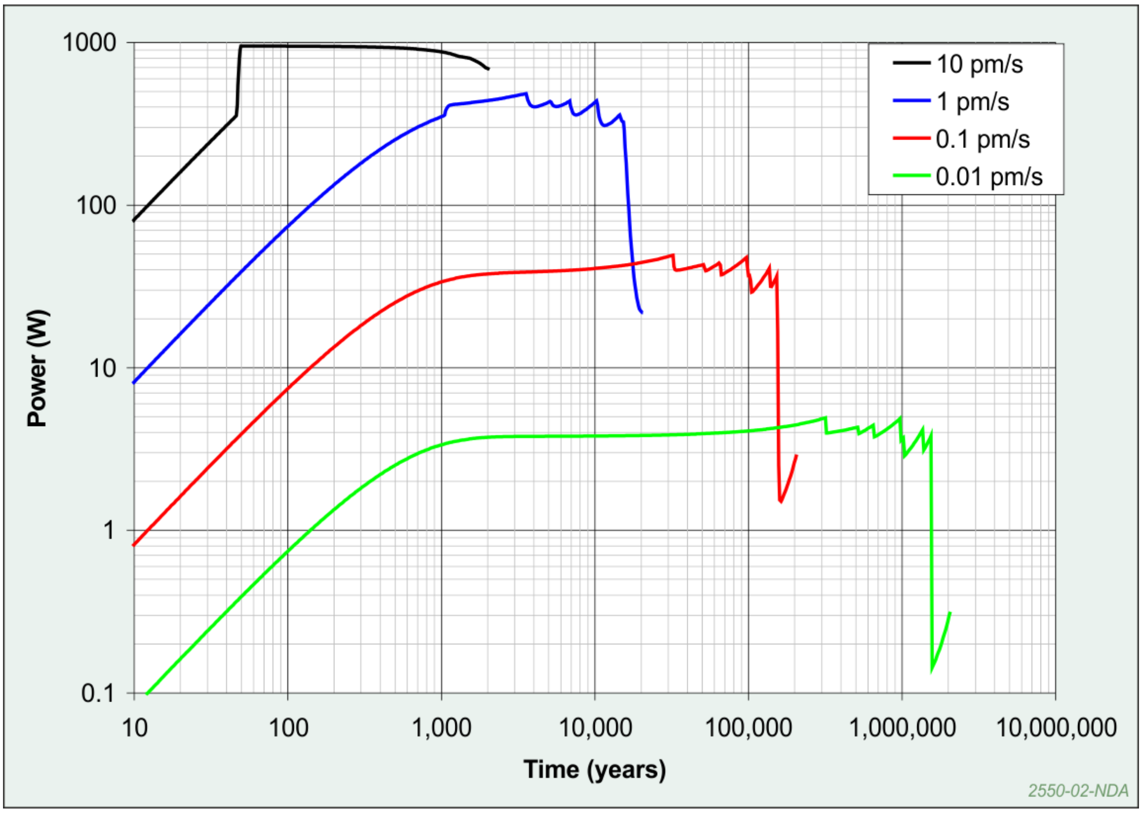


Figure 31 Power as a function of time for stack slumping of 7 kg of ^{235}U in 75% porous grout. 1 pm/s = 10^{-12} m/s for the slumping rates [76].



6.3.3 An in-package scenario for SF disposal

A criticality following spent fuel container failure and flooding is only credible for waste packages that contain fresh or low burn-up fuel. Only a quasi-steady state critically could occur and the consequences of such an event are calculated to be a temperature rise of 165°C and a power of less than 2000 W.

As a representative in-package scenario for SF disposal, the flooding of a package containing PWR fuel disposed of vertically in a HSR geology can be considered[39]. It is assumed that, following the failure of the package container, water would enter the compartments containing fuel. For geological disposal the fuel is expected to be irradiated (burned up) from its use in a nuclear reactor. However, fresh fuel has also been considered as the expected worst case, in terms of reactivity insertion from interaction with water.

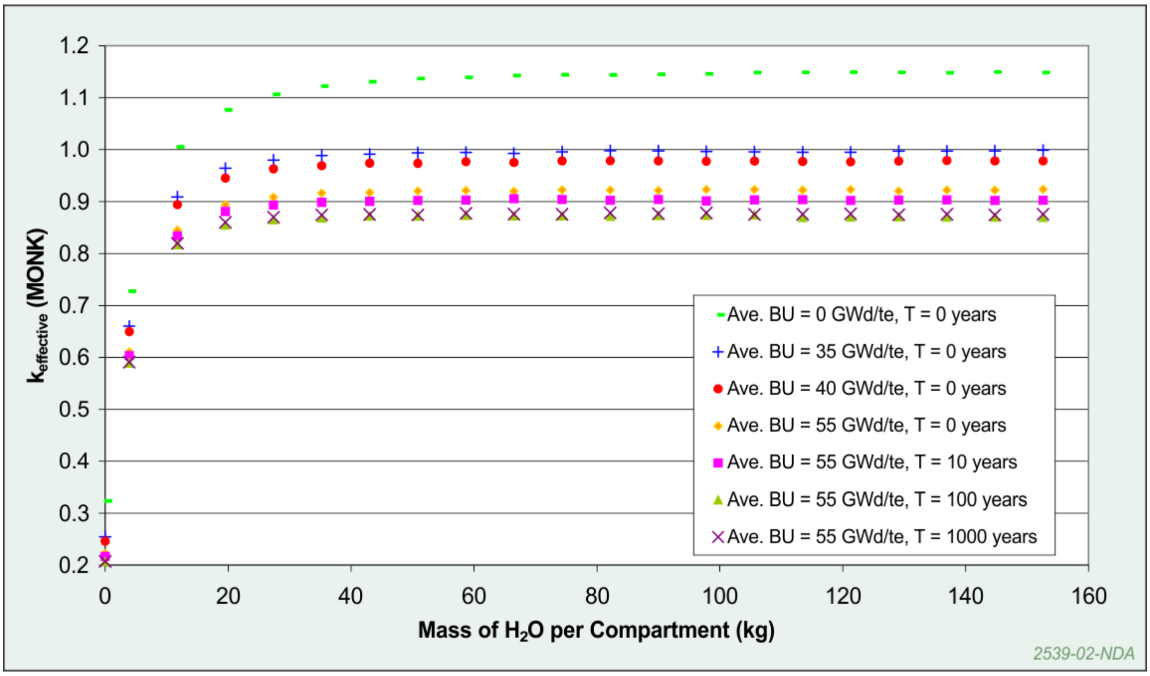
Analysis of this scenario used a geometrical model adapted from [26]. Criticality analysis for different volumes of flooding within the fuel compartments has been undertaken for fresh and irradiated PWR fuel in order to understand whether critical configurations are possible from flooding and, if so, how this changes with fuel irradiation. Where used, the irradiated composition is derived to include variation along the axial length of the fuel elements [95]. Figure 32 shows the results in terms of $K_{effective}$ (how close the flooded package is to a potentially critical system). The average irradiation is given in GWd/tU, and the cooling period, T, is given in years where applicable. 10 kg of water per compartment is equivalent to a flooded height of 0.289 m (156.5 kg = fully flooded). The figure shows that

[39] Both vertically (HSR) and horizontally oriented (LSSR) spent PWR fuel packages could, become critical, following partial package flooding with water. However, they would not become critical from flooding if the average irradiation of each fuel element is greater than 35 GWd/tU.

for fresh (zero irradiation) fuel the system can become critical with water ingress of approximately 11 kg per compartment. This is consistent with the analysis in [26]. For further water ingress the fresh fuel system reaches a peak $K_{effective}$ of about 1.15.

Figure 32 also shows that as the irradiation of the fuel increases, the possibility of a critical configuration reduces. At an average fuel irradiation of 35 GWd/tU it is just about possible to reach a critical configuration, while at higher irradiation levels the system remains sub-critical, even if the compartments containing the fuel elements are completely flooded. Furthermore, at an average irradiation of 55 GWd/tU, calculations allowing for different cooling periods (which can be compared with the time from taking the fuel out of a reactor to the onset of flooding of a container in the GDF), it can be seen that cooling acts to make the system even more sub-critical. The general conclusion from these calculations is that the formation of a critical configuration in a PWR SF container would not be possible provided that the average irradiation of all fuel elements in the container was above a modest 35 GWd/tU, meaning that we could take some conservative credit for the fuel irradiation history, a process referred to as actinide only burn-up credit[40]. Furthermore, if criticality did occur, for example due to the disposal of fresh PWR fuel, only a QSS transient would be possible.

Figure 32 Calculations of $K_{effective}$ as a function of water ingress into a spent PWR fuel disposal package (Variant 1, copper container) for fuel compositions at different levels of irradiation of initially 5% enriched uranium [95]



QSS calculations

For hypothetical critical systems initiated from partial flooding of a package containing fresh PWR fuel the temperature feedback coefficients are negative, so that only quasi-steady-state critically events could be considered with continued flooding/moderation acting as the reactivity insertion mechanism. QSS calculations were undertaken for an initial system

40 The actinide only burn-up credit approach allows credit for the changes in the ^{234}U ^{235}U, ^{236}U, ^{238}U, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu and ^{241}Am concentration with burnup. No credit for fission product neutron absorbers is taken.

corresponding to the just-critical point for the zero irradiation curve in Figure 32. A wide range of flooding rates from 10^{-14} m/s (~14.3 million years to flood the fuel compartments) to 10^{-3} m/s (1.25 hours to flood the compartments) were considered since, dependent on the mechanism for flooding, the rate could be relatively fast (for example, shearing of the container following geological activity) to very slow (such as slow water ingress due to pin-hole corrosion through the container and insert). It is difficult to judge which of the rates (if any) would be the most likely.

The results of a set of QSS calculations for different rates of flooding are given in Figure 33 and Figure 34. Thermal conduction through bentonite was assumed for heat transfer. For the flooding rates 1 pm/s = 10^{-12} m/s, at the lowest flooding rates the results show that an increase in the flooding rate by a factor of ten increases the power and temperature by a factor of ten. At higher flooding rates (10^{-11} m/s and larger) the behaviour is different. The explanation for this is that were the water to boil, no critical configurations would be possible. Since a quasi-steady-state criticality requires a continued just-critical configuration, the temperature must be limited to values below the boiling temperature of water. In fact, for all of the larger flooding rates, the temperature is bounded by 205°C (a temperature rise of 165°C) and the power is less than 2000 W. To put these values into context, these power levels are comparable with those expected during the earlier stages of SF disposal where the radioactive decay of activated materials and fission products would produce heat within the waste packages which would lead to temperature increases in the container and the surrounding buffer. Figure 13 in [2], for example, shows a temperature rise of up to about 80°C over a period of a few thousand years post-closure for a SF canister based on a Canadian SF disposal concept.

Figure 33 Average temperature increase of the fissile material region as a function of time for an in-package scenario for a PWR fuel disposal container (Variant 1). Adapted from [95].

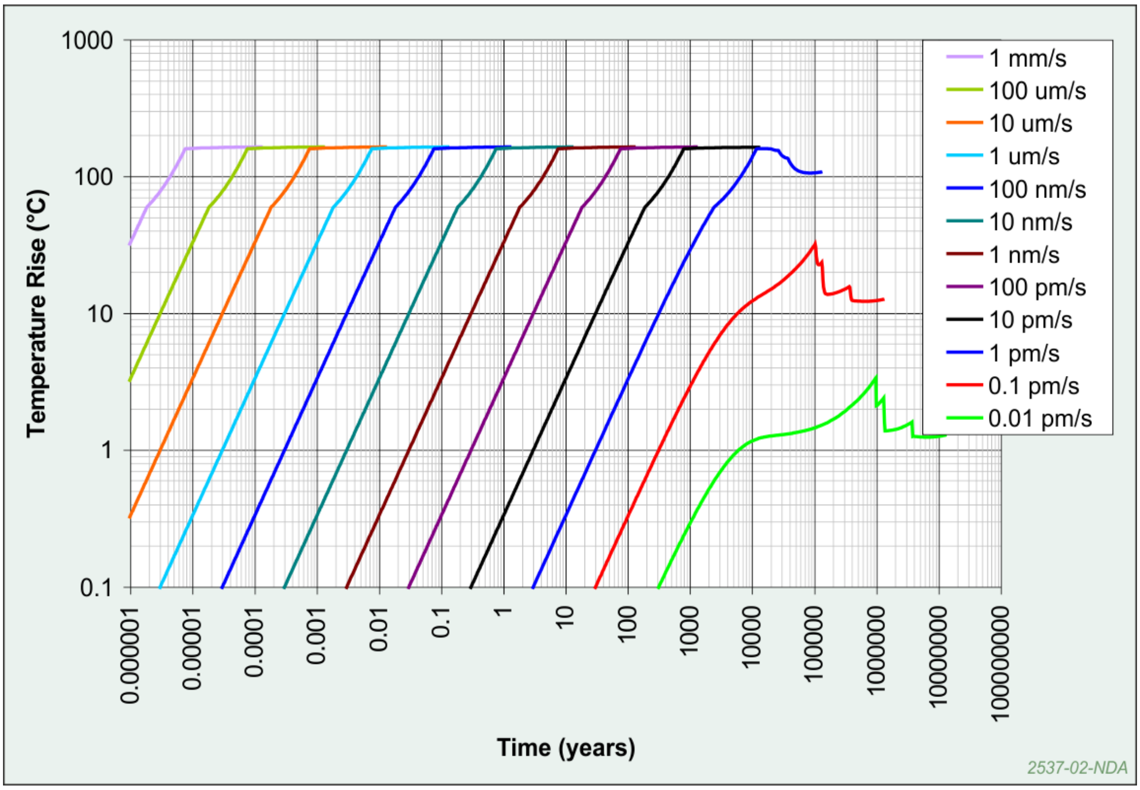
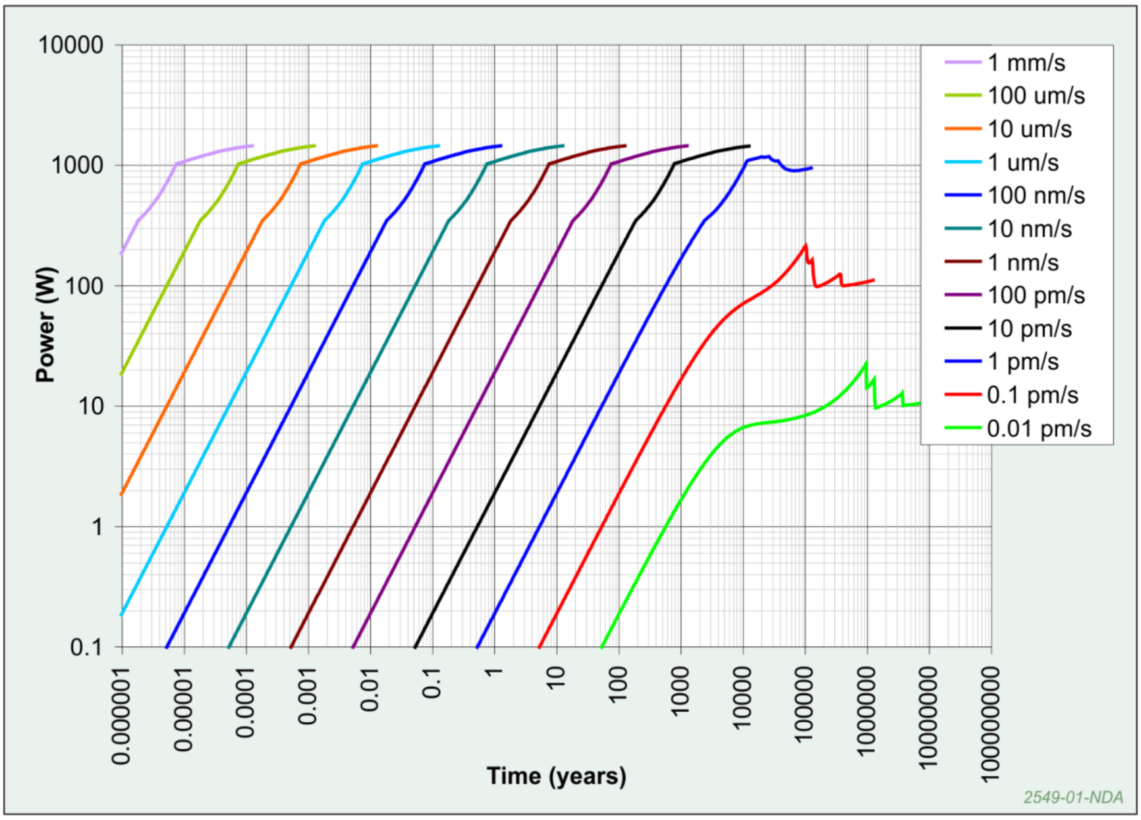


Figure 34 Power as a function of time for an in-package scenario for a PWR fuel disposal container (Variant 1). Adapted from [95].



6.3.4 An in-package scenario for plutonium and HEU disposal

The ceramic wasteform and can-in canister packaging concept for plutonium and HEU is inherently safe with regards to criticality. No in-package critical configurations were found.

As a representative in-package scenario for plutonium and HEU disposal, the removal of neutron absorbing materials has been considered for the can-in-canister packaging concept. It is assumed that following the failure of the container, insert and the inner cans, water could enter the small gaps between the fuel pucks. If water could preferentially remove neutron absorbers then this could act to increase $K_{effective}$.

Analysis of this scenario used a geometrical model adapted from [26]. Criticality calculations were undertaken for plutonium (90 and 100 wt% ^{239}Pu, where any remaining plutonium is ^{240}Pu) and HEU (90 and 100 wt% ^{235}U, where any remaining uranium is ^{238}U) with a 0.01 cm gap between the pucks within the cans (being the only initial void space in the package) as either empty space or flooded with water. In all calculations the value of $K_{effective}$ was less than 0.1554, representing a significantly sub-critical arrangement. The largest value calculated was for 100 wt% ^{239}Pu with flooding of the small volume of void space between the pucks. The observation that $K_{effective}$ is significantly sub-critical for all arrangements considered is consistent with the analysis in [26].

Further calculations were then undertaken to see whether changes to the material compositions (specifically the removal of neutron absorbers) could increase $K_{effective}$ to a critical value. A set of increasingly pessimistic sequential studies were undertaken to understand the combined effects of removing different neutron absorbers. In each case the maximum value of $K_{effective}$ was for the ^{239}Pu system with water in any gaps in the package contents. The results for a number of changes are shown in Table 6. The table shows that even after the removal of several neutron absorbing isotopes and the removal of the glass surrounding the inner cans, the system is still significantly sub-critical. This suggests that the ceramic wasteform and its packaging concept are inherently safe with regards to criticality. Since no critical configurations were found for this scenario no transient criticality calculations were conducted.

Table 6 Summary of criticality calculations for changes to material compositions in plutonium and HEU packages. All changes are sequential [95].

Model and sequential change	Largest value of $K_{effective}$
Base model. Water in the gaps between the pucks.	0.1554
All boron isotopes in the borosilicate glass replaced by boron-11.	0.3232
All gadolinium isotopes in the ceramic fuel replaced by gadolinium-162.	0.3710
All hafnium isotopes in the ceramic fuel replaced by hafnium-176.	0.4187
Cracked and dissolved borosilicate glass (largest $K_{effective}$ for complete dissolution and removal of the glass).	0.5227

6.4 International experience in assessing the consequences of criticality

We have reviewed the international approaches to understanding the consequences of post-closure criticality. It is our understanding that the UK research is currently amongst the most advanced.

We have recently conducted a literature review of international treatments of hypothetical criticality consequences [38]. The scope of the review was to address only the potential consequences of a criticality event, should one be initiated, without regard to its likelihood. The review was also limited to potential consequences of post-closure criticality, not operational accidents.

Work conducted for each country is summarised separately. This is because most of the research has been done on a national basis, rather than as part of international programmes. Nevertheless, the findings from researchers in one country can inform the work carried out elsewhere, including the UK, even if the proposed disposal concept is different.

The review [38] starts with work carried out in the USA, where most of the early studies were carried out, and finishes with a brief summary of work done in the UK. Table 7 shows the key results from non-UK analysis of the consequences of criticality. The table summarises the geological environments considered for the analysis, the waste type(s) and whether consequence analysis was for hypothetical QSS or RT criticality events. Further information about these studies, including references, is provided in [38].

Table 7 A selection of (broadly) post-closure criticality consequence assessments made outside of the UK [38]

Country	Geology	Waste type	QSS or RT	Consequences predicted		
				No. of fissions	*Heat / energy yield*	*Physical damage*
USA	Soil (10m deep)	LLW	QSS	$4.1\ 10^{21}$	-	-
USA	Salt bed	TRU waste	RT, QSS	$\sim 10^{27}$	Low	'Negligible'
USA	Unsaturated tuff	HEU, SF	RT, QSS	10^{20} (bounding) 10^{25} over 10,000 years	Insignificant	Void radius 1.4 m
USA	Unsaturated tuff	SF	QSS	-	100 W	-
France	Clay	SF	QSS	$1.3\ 10^{26}$	Fuel at 230 °C	None
Sweden	Hard rock	SF	QSS	-	20 kW Fuel at 265 °C	-

6.5 Conclusions and key assumptions

Understanding and demonstrating the consequences of hypothetical post-closure criticality is considered to be a mature research area, considering the generic stage of GDF development that the UK programme is currently at. We foresee minimal further research requirements until we reach a site-specific stage of GDF development.

To understand the potential consequences of hypothetical post-closure criticality events a significant programme of research has been undertaken. This programme identified that two types of transient criticality event could, hypothetically, develop:

- quasi-steady-state, where a just-critical system could be maintained over a period of time
- rapid transient, characterised by a short lived energetic release.

Software models of how hypothetical critical events could evolve have been developed – the QSS model and the RTM. For the latter a Bounding Approach model was also developed as a simpler alternative.

Initially, the application of these models focussed on the 'what-if' scenario of post-closure accumulation (transport of fissile radionuclides to a localised critical volume) from the disposal of ILW in the GDF located in a higher strength rock environment. More recently, the QSS model and Bounding Approach model have been applied to scope the consequences of hypothetical criticality transients in other materials (now covering all higher activity materials) and the three illustrative host rocks and relevant concepts.

The analysis of the ‘what-if’ scenarios included static criticality analysis to determine whether different configurations of fissile material could be critical (although expected to be very low likelihood) or whether criticality is not possible.

Box 12 summarises the static criticality analysis work conducted to assess the consequences of post-closure criticality.

Box 12 Summary of static criticality analysis work to assess consequences of post-closure criticality

Static criticality analysis has shown:

- for the accumulation scenario, critical masses are hypothetically possible in grout, NRVB, bentonite, granite and clay, but not in evaporite. The mass of fissile material required for a critical configuration would require the contents of multiple packages for some waste types, including HLW. The majority of hypothetical criticality events from fissile accumulation would evolve as quasi-steady state transients. Rapid transient criticality is only, hypothetically, possible over a narrow range of ^{239}Pu concentrations.

- for the stack slumping scenario, critical configurations are only possible if the encapsulant grout is sufficiently degraded and there are kilogram quantities of fissile radionuclides that can slump together. Package degradation leading to slumping would have to occur on a timescale of less than 100,000 years for rapid transient criticality to occur, since sufficient ^{239}Pu mass is required for a rapid transient criticality, and the mass of ^{239}Pu reduces with time due to decay.

- in-package scenarios are only credible for waste packages that contain sufficient fissile mass and would require partial or complete flooding with water or significant rearrangement following degradation. Based on the fissile content of individual packages such scenarios are conceivable (but considered very unlikely) for a small number of ILW and LEU packages, fresh or low burn-up SF, plutonium and HEU, but not LLW or HLW.

For potential critical configurations our analysis has also determined whether the system would become more or less critical with an increase in temperature; transient criticality analysis using the RTM or the Bounding Approach model has been applied to the former, and the QSS model to the latter.

Rapid transient criticality calculations have been undertaken using the Bounding Approach model for hypothetical criticality events from the accumulation and stack slumping scenarios. Box 13 summarises the key conclusions from the rapid transient criticality analysis conducted to assess consequences of post-closure criticality.

Box 13 Summary of rapid transient criticality analysis conducted to assess consequences of post-closure criticality

- Rapid transient criticality could only occur for a narrow range of hypothetical conditions. Such a criticality is not considered to be credible after about 100,000 years post-closure.
- no in-package scenarios that could evolve as rapid transients have been found.

Conclusions from the rapid transient analysis are:

- considering 10 kg of fissile oxide mass for accumulation, the Bounding Approach model predicts an energy release that could create a local cavity radius of no greater than 6.2 m. Local cracking would extend to no more than a few tens of metres. Larger mass accumulations, which are considered less likely, and would initially take longer to accumulate, would have larger consequences. However, the relationship is weaker than linear; for example, increasing the mass of $^{239}PuO_2$ by a factor of ten scales the cavity radius by a factor of about three. The relationship is weaker still if the decay of ^{239}Pu is taken into account, since for a given fissile mass the consequences reduce as ^{239}Pu decays to ^{235}U.
- stack slumping calculations with 7 kg of fissile oxide demonstrate similar consequences to the 10 kg accumulation calculations.

Quasi-steady-state transient criticality calculations have been undertaken using the QSS model for the accumulation scenario, stack slumping scenario and the in-package scenario of water flooding a fuel package containing fresh PWR fuel. In all cases the criticality events need a mechanism to sustain them, such as continued arrival of fissile material, continued slumping, or continued flooding. Calculations have been undertaken for a range of values (rates) for the sustaining mechanisms.

Box 14 summarises the QSS transient criticality analysis work conducted to assess consequences of post-closure criticality.

Box 14 Summary of QSS transient criticality analysis conducted to assess consequences of post-closure criticality

Conclusions from the QSS transient analysis are:

- for a wide range of fissile material arrival rates in the accumulation scenario, slumping rates in the stack slumping model, and flooding rates for an in-package scenario, the power of the transient criticality events would be limited to a few kilowatts, and localised temperature rises (of the critical region) would be limited to less than 300°C.
- furthermore, where the temperature distribution into the surroundings is calculated, temperature rises of more than 10°C above ambient are limited to a localised radius of a few metres.
- for the accumulation scenario larger consequences are possible at higher rates of fissile material accumulation, but only if it is assumed that accumulation can continue when the pore water boils. Porewater boiling will however generally act to not only prevent accumulation of fissile material, but also acts to reduce neutron moderation.

All of the results demonstrate that hypothetical post-closure criticality would have limited local, physical consequences on the GDF and that it therefore does not pose a significant concern. Section 7 of this report discusses how we link these local physical consequences to their potential impact on post-closure performance. By doing this we seek to fully demonstrate that post-closure criticality is not a significant concern.

We consider that, for the current phase in planning for the GDF, sufficient model development and analysis have been undertaken for the consequences of criticality to meet the requirements of the generic post-closure safety case.

7 Potential Impact on Post-closure Safety

This section of the report links the research on the likelihood and possible consequences of hypothetical post-closure criticality to the implications for post-closure safety, by discussing the approach used to assess the impacts on pathways in the post-closure safety case that may give rise to a risk.

A complete assessment of post-closure criticality safety will only be possible once site-specific details of the GDF are available. In the meantime, it is considered prudent to use the developed knowledge base and calculation methods to carry out generic preliminary assessments. RWM has undertaken an extensive programme of research with the objective of demonstrating that post-closure criticality will not be a significant concern. The approach taken to address the GRA requirements has been to consider, through both reasoned arguments and detailed numerical modelling:

- the likelihood of post-closure criticality (see Section 5)
- the consequences of post-closure criticality in the vicinity of hypothetical criticality events, including the use of a ‘what-if’ approach coupled with arguments of credibility (see Section 6)
- the assessment of how hypothetical criticality events could impact on the baseline post-closure performance of the GDF. This is the role of the methodology discussed within this section. Results from the application of this methodology are summarised within our generic post-closure safety assessment [15].

From the likelihood of criticality work, it is argued that criticality is only credible within assessment timeframes under specific circumstances and, if it occurred, it would be at very long times into the future:

- criticality is not considered credible in the normal evolution of the GDF in an evaporite geology due to negligible flow rates, very low porosity and the chemical composition (chlorine is an effective neutron absorber)
- a post-closure RT criticality is not considered credible for any waste types or geological environments.

The situations in which a QSS criticality could be considered credible are:

- in ILW vaults in higher strength rock, for waste types with relatively high masses of fissile material, at timescales of hundreds of thousands of years after closure or later
- criticality associated with fresh (un-irradiated) fuel or low burn-up SF in the GDF in higher strength rock or lower strength sedimentary rock
- criticality due to the accumulation of fissile material from plutonium or HEU in the GDF in higher strength rock or lower strength sedimentary rock (on timescales of longer than one million years).

It is emphasised that, while there are circumstances for which criticality cannot yet be argued to be impossible, this does not mean that it is considered to be likely.

7.1 Approach to generic post-closure criticality consequences assessment

Sufficient knowledge now exists to allow understanding of the likelihood and local physical consequences of post-closure criticality to support the generic post-closure safety assessment. The effects on post-closure safety of even the largest (and intuitively most unlikely) 'what-if' criticality events would be modest and tolerable for the GDF.

The generic post-closure criticality consequence assessment (PCCCA) [96] summarised in this section has been conducted to fulfil the 'what-if' analysis that is a requirement of the GRA [20]. That is, criticality events which are not considered credible are assessed, as well as criticality events which could, on the basis of current understanding, conceivably occur. When undertaking a 'what-if' assessment, it is still necessary to make a judgement about how implausible the scenarios considered are. The scenarios assessed were developed at an expert workshop, where it was agreed that:

- the focus of the assessment would be on higher strength rock and lower strength sedimentary rock (based on arguments about the negligible likelihood of criticality in the GDF in evaporite)
- the largest RT criticality events considered would assume 10 kg of fissile material (since an RT criticality of any size is not considered credible, and they become less likely as increasing amounts of fissile material are involved)
- the possibility of multiple independent criticality events would be neglected (given the low likelihood of a single criticality occurring).

RWM previously undertook a post-closure criticality consequences assessment in 2008 [97]. The 2008 PCCCA was a key reference in supporting our argument that the possibility of a post-closure criticality event in the GDF will not be a significant concern and that the consequences of any hypothetical criticality on GDF performance would be limited. Since this time we have developed the 2008 PCCCA by adding more detail and expanding the range of disposal concepts considered, in order to more robustly underpin the position that post-closure criticality is a low likelihood and low consequence event. Compared to the 2008 PCCCA, the 2015 version included:

- recent work on the likelihood and consequences of criticality; this was particularly the case for the likelihood work. The understanding developed in this work was used to refine the scenarios considered in the post-closure assessments. In particular the 'large' RT criticality events involving hundreds of kilograms of fissile material considered previously were discounted as not credible in the 2015 assessment, even as 'what-if' scenarios. Information about the properties and localised consequences of a criticality were taken directly from the recent consequences research.
- the PCCCA is now based on the 2010 DSSC. The DSSC forms the baseline against which the impacts of a criticality are considered.
- the range of waste types considered was extended to cover all higher activity waste.
- refinements were made to assessment methodologies, including a more explicit representation of a hypothetical criticality in assessment models of radionuclide transport. To address the GRA requirement to consider 'what-if' scenarios and in response to peer-review challenge, consideration of the consequences of inadvertent human intrusion was also extended in scope to consider the potential for the intrusion to increase the likelihood of post-closure criticality.

The primary effects of a criticality with the potential to impact GDF performance were identified as:

- increased temperature
- increased pressure
- changes to the inventory of radioactive material
- increased radiation levels.

Each of these primary impacts was considered in terms of their ability to compromise barriers in the GDF that form the basis of the safety case. The assessments summarised in this section used the 2010 DSSC [98], and in particular the post-closure safety assessment [99], as a baseline as far as possible. Following the approach in [99], the effects of criticality on GDF post-closure performance were considered in the following categories:

- the transport of radionuclides in groundwater (the groundwater pathway)
- the transport of radioactive gas and other potential effects of GDF-derived gas on post-closure performance (consequences of gas)
- the consequences of inadvertent human intrusion (the human intrusion pathway)
- the transport of chemically toxic materials in groundwater (chemotoxic assessment).

Key conclusions from the assessments are presented within our updated post-closure safety assessment [15], which highlights that even when using pessimistic assumptions for the occurrence and local consequences of hypothetical criticality, such events do not have a significant impact on the assessed post-closure GDF performance.

7.2 Conclusions of generic post-closure criticality consequences assessment

Our generic post closure criticality consequences assessment has demonstrated that, in the unlikely event of a post-closure criticality occurring, the consequences would not significantly degrade the post-closure performance of the GDF.

The consequences of post-closure criticality are limited because:

- QSS criticality events are likely to affect only a limited part of the GDF’s volume in terms of elevated temperature and radiation levels
- RT criticality events with fissile masses of up to 10 kg might have a significant localised impact on the GDF and the engineered barrier system, but these events would not be expected to significantly damage the geosphere barrier
- for the disposal concepts and geological environments assumed in this generic assessment, the geological barrier will still act to isolate the radioactive waste from the surface environment, even if localised parts of the EBS are damaged
- the change in inventory associated with criticality is modest in comparison with the original inventory for disposal
- criticality is only considered credible at very late times, by which time the inventory of some key radioactive isotopes, such as ^{14}C, will have decayed and the inventory of reactive metals would be exhausted, reducing the gas-related consequences of any hypothetical criticality event.

A complete assessment of criticality safety will only be possible once site-specific details of the GDF are available. However, considering the likelihood research (see Section 5), consequences research (see Section 6) and the post-closure performance assessment work summarised within our post-closure safety assessment [97], it is expected that post-closure criticality:

- would have a low probability of occurrence, or would not be credible at all
- would not have a significant impact on GDF performance, even for pessimistic assumptions about both the occurrence and evolution of a range of ‘what-if’ criticality events.

8 Summary and Conclusions

We have produced this report to document the knowledge base that supports the three safety cases for demonstrating criticality safety (transport, operational and post-closure). Most of our criticality safety work has historically been on LHGW (primarily ILW); but our remit is now broader and we now consider all higher activity materials destined for geological disposal. We also summarise the current understanding of criticality safety for HLW, SF, plutonium and uranium.

Currently there are uncertainties about the nature of the site and the design of the disposal system, because a site has not yet been selected. Therefore we are developing a generic geological disposal design to provide the basis for planning. As planning progresses details of the final packaging, emplacement and geological environment conditions will become available. We will therefore continue to update the safety assessments to ensure that criticality safety requirements are fully considered.

8.1 Transport and operational phases

We deterministically demonstrate that that a criticality accident is not credible based on multiple diverse barriers. We assess criticality safety as part of the safety cases that we are producing for waste transport and operation of the disposal facility. We also assess criticality safety as part of our advice to waste producers on conditioning and packaging proposals.

The following contributions to safety apply based on our understanding of how the waste packages and the GDF will evolve over time.

For the waste material:

- RWM has a detailed knowledge of the inventory of radioactive wastes and materials based on a set of assumptions derived from government policy and our understanding of future wastes.
- for the majority of the wastes criticality safety is not a concern. In ILW the fissile material is nearly always mixed with a large excess of non-fissile material. HLW contains little fissile material because this has been separated in reprocessing of SF.
- small amounts of ILW will contain separated plutonium and HEU, but these are not present as pure materials – they are dispersed amongst other non-fissile waste materials.
- for pure materials such as plutonium and HEU, RWM can design a stable wasteform that is sub-critical, as in the current packaging assumption; for example, our research has indicated that the assumed wasteform for plutonium would remain sub-critical on omission or loss of neutron absorbing materials from the ceramic wasteform. Depleted and natural uranium are not classed as fissile material.
- although RWM often conservatively applies a ‘fresh fuel’ assumption to SF for transport and operational phase criticality safety assessment, in reality, most SF is removed from nuclear reactors because a large proportion of the fissile content has been used up during irradiation. For example, our research has indicated that for PWR SF in a disposal container, ingress of water would not result in criticality for fuel assemblies irradiated to burn-ups in excess of 35 GWd/tU (the average burnup for legacy SF is 45-55 GWd/tU).

For the packages:

- RWM specifies and ensures control of all waste package contents.
- for the majority of SF, the wasteform design is already fixed, that is, it comprises a metallic or ceramic fissile material surrounded by cladding. So we will use a package design to ensure safe sub-critical conditions (for example, this might include using materials that absorb neutrons to prevent criticality).
- for packaging of HEU and plutonium at high loadings (as in the current packaging assumption of a ceramic wasteform emplaced in the HLW disposal area), contributions to safety will be provided by a stable, sub-critical wasteform and a long-lived container.

In all cases RWM aims to design packages that are robust to faults during transport and operations. We use well established methods with appropriate conservatisms. In some cases we are able to apply methods used by waste producers to produce packages already stored under existing approved site safety cases. In the Disposability Assessment process, we ensure that these packages are properly designed by assessing them against waste package specifications. We also use the Disposability Assessment process to help ensure that the packages actually produced meet these specifications. In time, we will replace these specifications with Conditions for Acceptance.

8.2 Post-closure phase

Criticality safety is also assessed as part of the assessment of post-closure risks. Depending on the type of waste, we design the packages to contain their fissile material for medium to long timescales. Over extended times, the packages will degrade as the containers resaturate and corrode and a portion of the package contents may become mobilised by groundwater. We consider a post-closure criticality to be unlikely; a low probability event. However with large numbers of packages and very long timescales it is difficult to guarantee that a criticality cannot occur (that is, to demonstrate zero likelihood). Therefore we have carried out research to understand how a criticality could begin, progress and end, and what the physical consequences would be. We apply the following safety arguments to the consideration of post-closure criticality safety.

The likelihood of post-closure criticality is low because:

- waste containers will be emplaced in the GDF in a sub-critical configuration with multiple engineered barriers in place to retard the effects of processes that might lead to significant relocation of fissile material.
- many of the anticipated changes in the evolution of waste packages in this environment following closure are expected to reduce system reactivity.
- for ILW, the fissile material is well spread out; the total fissile content of 13.5 tonnes dispersed through ~470,000 m^3 of waste packaging materials, at concentrations well below critical values.
- the majority of ILW is/will be encapsulated in cement, and ILW disposal concepts are based on cementitious backfill, the chemical and physical properties of which hinder movement of fissile material.
    - our likelihood research relating to the disposal of LLW/ILW/DNLEU has found that criticality is not credible when considering most ILW packages. Conditions required for criticality were calculated to be met in only about 2% of the probabilistic realisations for the higher strength rock disposal concept. The conditions of concern can generally be traced back to specific waste packages with a high fissile material content, which represent just under 2%

of unshielded ILW packages for which designs have not yet been assessed in the Disposability Assessment process.

- in the lower strength sedimentary rock disposal concept, where movement of fissile material will be by diffusion in water, and in the evaporite disposal concept where there is assumed to be no water present, conditions remain sub-critical.

- for pure plutonium and uranium materials, which are not yet categorised as wastes, RWM could design a wasteform that is stable for long times and would only very slowly release fissile material, as in the current packaging assumption:
    - In RWM's likelihood research, calculations indicate that failed HEU/plutonium packages would remain sub-critical because of the neutron absorbing components of the wasteform. Sufficient ^{235}U from HEU/plutonium packages could accumulate in the surrounding buffer to support criticality on timescales in excess of 10^6 years, although the accumulated masses have been compared with the critical masses of idealised spherical configurations, which are not considered to occur naturally and may be overly cautious.
- for SF we will use a package and emplacement design capable of maintaining sub-critical conditions over very long timescales and, in the majority of fuel types, the reactivity will reduce with time as ^{239}Pu decays into the less reactive fissile nuclide ^{235}U, both of which will be diluted by the non-fissile ^{238}U.
    - in RWM's likelihood research, calculations indicate that AGR and PWR SF in high-integrity containers will always be sub-critical under water-moderated conditions provided the average irradiation of the fuel is above a certain amount (for example 35 GWd/tU for PWR SF). The calculations indicate that insufficient uranium for criticality would accumulate in the buffer surrounding a failed container up to very long times (after 10^8 years) in the higher strength rock concept.
    - in the lower strength sedimentary rock disposal concept, shorter container lifetimes have been assumed. As a result, greater masses of uranium are calculated to migrate into the buffer. The modelling indicates that enough ^{235}U could accumulate in the buffer surrounding a failed PWR container to challenge the minimum critical mass in bentonite (when compared to an idealised water-moderated spherical configuration, which is not considered to occur naturally) if the accumulated uranium derives from fresh PWR fuel.

The consequences of a post-closure criticality are low because:

- rapid transient criticality could only occur for a narrow range of hypothetical conditions, and that such a criticality is not considered to be credible after about 100,000 years post-closure, due to decay of ^{239}Pu to ^{235}U.
- for a QSS criticality, the physical consequences are highly localised and would not be expected to affect the surrounding geosphere and therefore would not significantly impact overall risk.
- direct radiation from a criticality event would be shielded by the surrounding rocks and materials. Unlike during the transport or operational phases of the GDF there would be no direct risk posed to operators or members of the public.
- for QSS criticality, the calculated temperature rise and power are less than 300°C very locally and a few kilowatts, irrespective of whether the underlying scenario is accumulation, stack slumping or in-package flooding.

- even if such were to occur, criticality events are likely to affect only a limited part (of the order of tens of cubic metres) of the GDF.
- criticality events involving very large amounts of fissile material might have a significant impact on a small fraction of the GDF and the engineered barrier system, but these events are very unlikely and could only occur a long time (hundreds of thousands of years) after closure, when the radioactive inventory will have decayed to much lower levels. Therefore their effect on the overall risk will be small.
- the backfill/buffer and geological environment will still act to isolate the radioactive waste from the surface environment.

Based on the modelling of the consequences of possible criticality events, and combining this with estimates of their likelihood, we consider that the risk from post-closure criticality is not a significant concern.

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