Scientific Basis for a Safety Case of Deep Geological Repositories

GRS - 501

Gesellschaft für Anlagen-
und Reaktorsicherheit
(GRS) gGmbH

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Zusammenfassung

Die in diesem Projekt durchgeführten Arbeiten haben zu verschiedenen Aspekten eines Safety Case einen Beitrag geleistet; speziell zu den Nachweisgrundlagen (Prozessverständnis), zu den Methoden und Strategien zur Entwicklung eines Safety Case, zur Langzeitsicherheitsanalyse und zu zusätzlichen Nachweisen, Analysen und Argumenten, die in einem Safety Case verwendet werden. Laufende nationale und internationale Entwicklungen wurden verfolgt und diskutiert. FuE-Projekte mit Relevanz für die Langzeitsicherheit von Endlagern für radioaktive Abfälle wurden analysiert und bewertet um das Prozessverständnis zu erhöhen. Sofern möglich, wurden neue konzeptuelle Modelle und/oder Parametersätze für die Langzeitsicherheitsanalyse vorgeschlagen.

Die Entwicklungen in anderen Ländern und auf internationaler Ebene wurden verfolgt durch Teilnahme an internationalen Komitees und Arbeitsgruppen, wie dem Radioactive Waste Management Committee (RWMC), der Integration Group for the Safety Case (IGSC), dem Clay-Club, Salt Club, Crystalline Club sowie Aktivitäten der IAEA zur Behandlung der Biosphäre in einem Sicherheitsnachweis. GRS war z.T. federführend involviert in Arbeitsgruppen und Topical Sessions, in denen der Status sicherheitsrelevanter Aspekte eines Safety Case für tiefe geologische Endlager (DGR) bewertet und Methoden und Vorgehensweisen weiterentwickelt wurden. IGSC Topical Sessions zu den Themen (i) Relevanz von Gasen in einem Safety Case, (ii) Rolle und Verwendung geowissenschaftlicher Argumente bei dem Standortauswahlprozess und (iii) Kritikalität und Safeguards in einem DGR wurden organisiert, ausgewertet und zusammengefasst. Diese Topical Sessions geben den derzeitigen Stand zu dem jeweiligen Thema in den NEA Mitgliedsstaaten wieder und repräsentieren damit einen großen Erfahrungsschatz. Dieses Wissen liefert einen tieferen Einblick in Aspekte des Safety Case und kann Anregungen zur Überprüfung und Weiterentwicklung nationaler Methoden und Vorgehensweisen beitragen.

Ein derzeit wichtiges Thema, das auch in Arbeitsgruppen der NEA (Nuclear Eergy Agency) thematisiert wird, stellt die Kommunikation des Safety Cases dar. Zwei Aktivitäten, die von deutscher Seite wesentlich unterstützt wurden, sollen hier herausgestellt werden; zum einen die Kommunikation komplexer technischer Inhalte eines Safety Case mit der Öffentlichkeit, speziell technisch nicht ausgebildeten Personen, zum anderen die Fragestellung, wie Aufzeichnungen und Dokumente, Wissen und Erinnerungen über ein Endlager für radioaktive Abfälle nach dessen Verschluss für zukünftige Generationen erhalten werden kann. Die erste Aktivität wurde von einer IGSC Arbeits-

gruppe durchgeführt. Basierend auf einem Review von internationalen Projekten, Initiativen und lokalen Veranstaltungen zur Kommunikation von Themen zur Endlagerung radioaktiver Abfälle wurden effiziente Ansätze und Strategien zur Kommunikation herausgearbeitet. Schwierigkeiten und Herausforderungen bei der Kommunikation wurden beschrieben und Ideen zur Verbesserung der Kommunikation präsentiert.

Die zweite Fragestellung wurde im Rahmen der NEA Initiative „Preservation of Records, Knowledge and Memory (RK&M) Across Generations“ behandelt. Geologische Endlager beruhen auf einer sogenannten passiven Sicherheit und bedürfen nach ihrem Verschluss keiner weiteren Wartung bzw. keiner menschlichen Eingriffe. Allerdings ist es nicht beabsichtigt, diese Endlager bzw. das Wissen darüber zu vergessen. Vielmehr sollen Dokumente und Aufzeichnungen, Wissen und Erinnerungen zu einem Endlager so lange wie möglich erhalten werden und damit dazu beitragen unbeabsichtigtes menschliches Eindringen in das Endlager zu vermeiden sowie zukünftigen Generationen Entscheidungen hinsichtlich des Endlagers zu ermöglichen. In der Initiative wurde eine systemische Strategie bestehend aus einem Ensemble von Mechanismen und Ansätzen erarbeitet, die verwendet werden kann, um RK&M über Generationen zu erhalten. Im Rahmen des Projekts wurde insbesondere die Entwicklung des Ansatzes zum „Set of Essential Records“ (SER) unterstützt. Der SER ist zu verstehen als eine Sammlung der wichtigsten Dokumente und Aufzeichnungen über ein Endlager, die während des Endlagerprogramms für eine ausgewählt und für unbegrenzte Zeit erhalten werden sollen. Mit dem SER sollen ausreichend Informationen über das Endlager für jetzige und zukünftige Generationen zur Verfügung gestellt werden, damit diese ein angemessenes Verständnis des Endlagersystems haben, um die Entwicklung des Endlagers und den Safety Case verifizieren und überlegte Entscheidungen zum Endlager basierend auf der Bewertung der Konsequenzen treffen zu können.

Die Langzeitsicherheitsanalyse mit Berechnung der radiologischen Konsequenzen bildet den Kern eines Safety Case für ein Endlager für radioaktive Abfälle. Sie beinhaltet einen umfassenden Ansatz zur Behandlung aller Unsicherheiten, speziell der möglichen zukünftigen Entwicklungen eines Endlagersystems (Szenarios) mit den resultierenden, potentiellen Konsequenzen. Entsprechend der international bewährten Vorgehensweise basiert die Entwicklung von Szenarien für Sicherheitsanalysen für geologische Endlager auf FEP (Features, Events and Processes). Der Salt Club der NEA hat die Entwicklung einer internationalen FEP-Datenbasis für Endlager in Salzformationen initiiert. Die mittlerweile zur Verfügung stehende „SaltFEP“ Datenbasis ist über eine Internet-Plattform zugänglich und kann allen, die Szenarien für ein Endlager in Salz entwickeln wollen, Informationen über relevante Prozesse und Effekte in allen Kompartimenten eines Endlagersystems liefern. Zudem ist eine umfangreiche Referenzdatenbasis (das Salt Knowledge Archive) in der Datenbank hinterlegt.

In den letzten zehn Jahren wurden sowohl auf nationaler wie auch auf internationaler Ebene die Methoden zur Szenarienanalyse und -entwicklung erheblich weiterentwickelt und die Strategien modifiziert. GRS hat an einer Umfrage und einem Workshop der NEA-Arbeitsgruppe IGSC teilgenommen, bei dem die jüngsten Erfahrungen in den Mitgliedsländern der IGSC bei der Szenarienentwicklung und Behandlung von Ungewissheiten ausgewertet werden sollten. Die wesentlichen Ergebnisse sind in diesem Bericht dargestellt. Merklicher Aufwand wurde darin investiert, Szenarien möglichst umfassend, hinsichtlich aller Entscheidungen nachvollziehbar und mit möglichst logischer Strukturierung des interdisziplinären Wissens zu entwickeln. Die Szenarien und die Szenarienentwicklung werden heute in einem Safety Case deutlicher und umfassender dargestellt als früher unter Betonung der Transparenz und Nachvollziehbarkeit. Punkte, die einer Weiterentwicklung bedürfen werden zum einen in der Kommunikation der Rolle und der Auswahl von Szenarien mit der breiten Öffentlichkeit, zum anderen in der Zuordnung von Wahrscheinlichkeiten für die Szenarien gesehen. Die Behandlung unwahrscheinlicher Szenarien ist derzeit ein Arbeitspunkt der deutschen Arbeitsgruppe Szenarien. Unwahrscheinliche Szenarien beinhalten Entwicklungen mit einer Wahrscheinlichkeit kleiner 1 % und müssen analysiert und bewertet werden. Konsens der Arbeitsgruppe ist aber, dass es sinnvoll ist nur solche Szenarien zu betrachten, die eine Restwahrscheinlichkeit haben. Unrealistische Szenarien mit einer Eintrittswahrscheinlichkeit von null oder nahezu null sollten ausgeschlossen werden. Stattdessen ist die Betrachtung von „What-if Szenarien“ nützlich, um die Robustheit des Endlagersystems zu demonstrieren.

Generell ist neben den Ungewissheiten hinsichtlich der zukünftigen Entwicklung des Endlagersystems in einem Safety Case auch die Behandlung der Ungewissheiten bezüglich der verwendeten Modellparameter von hoher Relevanz. Diese Ungewissheiten können in den Sicherheitsanalysen direkt mittels deterministischer und/oder probabilistischer Ansätze berücksichtigt werden. Probabilistische Unsicherheits- und Sensitivitätsanalysen werden heute als ein essentielles Werkzeug bei der Analyse numerischer Modelle in Sicherheitsanalysen betrachtet. Speziell Sensitivitätsanalysen können wertvolle Informationen über das Modellverhalten liefern und damit zur Verbesserung des Systemverständnisses beitragen. Während des PAMINA-Vorhabens und danach wurden numerische Verfahren zur Sensitivitätsanalyse weiterentwickelt. Als Teil dieses

Projekts wurde eine Zusammenarbeit mit amerikanischen, belgischen und finnischen Teilnehmern ins Leben gerufen, um neuere Ansätze zur probabilistischen Unsicherheits- und Sensitivitätsanalyse zu vergleichen und Erfahrungen auszutauschen. Verschiedene Testfälle, die auf den jeweiligen nationalen Programmen basieren wurden für die Studie ausgewählt. Zum Zeitpunkt der Erstellung dieses Berichts liegen nur Ergebnisse orientierender Rechnungen von SANDIA und GRS vor. Sie zeigen, dass die Codes DAKOTA und RepoSUN sehr ähnliche Rang-Korrelationskoeffizienten berechnen, was als eine erste Verifizierung beider Codes angesehen werden kann. Trotz einer geringen Basis von nur 50 Spielen konnten beide Codes die sensitivsten Parameter im SANDIA-Modell für ein Endlager in Tonschiefer identifizieren. Diese Ergebnisse müssen allerdings auf Basis einer größeren Anzahl von Spielen bestätigt werden. Weiter Untersuchungen und Vergleiche unter Einbeziehung der Ergebnisse der belgischen und finnischen Gruppen sind vorgesehen. Dabei sollen Schlussfolgerungen zur Signifikanz der verschiedenen Methoden, der notwendigen Anzahl Spiele für verlässliche Sensitivitätsanalysen, der Einfluss der Komplexität sowie die Interpretation der Ergebnisse für die verschiedenen, betrachteten Endlagersysteme gezogen werden.

Hinsichtlich der Mobilität von Radionukliden wurde in Kooperation mit NAGRA eine Methode zur Ermittlung durchschnittlicher und maximaler Radionuklidinventare für verglaste Abfälle aus La Hague entwickelt und angewandt. Die Methode wird für Langzeitsicherheitsanalysen als akzeptabel betrachtet. Allerdings wäre es wünschenswert, auf internationale Ebene eine größere Anzahl von verglasten Abfällen einzubeziehen und eine Datenbasis für Radionuklidinventare zu erstellen, die die Genauigkeit der Daten weiter erhöhen würde.

Der wesentliche Teil der Arbeit zur Radionuklid-Mobilität bestand in der Beteiligung am EU-Projekt, CAST (Carbon-14 Source Term). Ziel des Vorhabens war es, ein besseres Verständnis zu möglichen Freisetzungs-Mechanismen von ^{14}C aus den Abfallmaterialien unter den relevanten Randbedingungen in einem tiefen geologischen Endlager zu entwickeln. GRS war an dem Arbeitspaket teil, in dem die Ergebnisse aus den experimentellen Arbeiten bezüglich des Endlagersystems bewertet und ihr Einfluss auf die Langzeitsicherheit analysiert wurde. Dazu wurde die vorläufige Sicherheitsanalyse Gorleben (VSG) als Grundlage verwendet. Es wurde ausschließlich die Freisetzung von ^{14}C aus Zircolay und Stählen betrachtet. Die Rechnungen zeigen, dass die Auswirkungen der ^{14}C Freisetzung, die als radiologischer Geringfügigkeitsindex (RGI) ermittelt wurden, zu frühen Zeitpunkten hauptsächlich durch die freigesetzte ^{14}C Menge bestimmt werden. Das zeitliche Verhalten der ^{14}C Freisetzung hat nur einen geringen Einfluss auf den Indikator RGI. Die Ergebnisse aus den Vorhaben CAST (und aus dem Vorhaben First Nuclides) zeigen, dass ein großes Potential zur Reduzierung der Konservativität bei der Behandlung von ^{14}C zu frühen Zeitpunkten in der Sicherheitsanalyse besteht. Diese Experimente deuten darauf hin, dass der Anteil des ^{14}C der instantan aus Zircaloy bzw. Stahl freigesetzt wird, in einem Bericht von 1 % liegt, und damit an der unteren Grenze der hier durchgeführten Variationsrechnungen und deutlich niedriger als der Wert von 10 %, der in der VSG im Referenzszenario verwendet wurde.

Im Rahmen des TDB Projekts (Thermodynamic Database) der OECD/NEA wird derzeit ein State-of-the-art Bericht zur geochemischen Modellierung von Löslichkeiten in hochsalinaren Lösungen unter Verwendung des Pitzer-Ansatzes angefertigt. Der Beitrag der GRS zu diesem Bericht umfasst die Analyse des derzeitigen Stands zu Eisen und Blei. Die Auswertung der vorhandenen Daten für zweiwertiges Eisen zeigt, dass Datensätze zum System $FeCl_2$ - Na, K, Mg, Ca - H2O existieren um Parameter für das Pitzermodell abzuleiten, für das entsprechende $FeSO_4$ System aber relevante Daten fehlen. Für die Ableitung eines Pitzermodells für dreiwertiges Eisen fehlen generell noch Daten und Experimente wie z.B. spektroskopische Messungen zur Quantifizierung relevanter Komplexe. Aufgrund der Vielzahl der bekannten Fe(III)-Komplexe wird empfohlen, entsprechende Experimente und mithin die Erstellung eines Pitzer-Modells auf solche Bedingungen zu beschränken, die relevant für ein Endlager sind.

Im Hinblick auf mikrobielle Effekt und Prozesse wurde die Review zu Endlagern in Ton und Salz weitergeführt. Für ein Endlager für wärmeentwickelnde Abfälle in Tonstein zeigte die Arbeit, dass für quantitative Abschätzungen der maximal möglichen, durch Mikroben verursachten Effekte ein entsprechendes Computerprogramm zwingend notwendig ist. Eine einfache Abschätzung ist nicht möglich, da das System konkurrierender bzw. synergistischer mikrobieller Subpopulationen, die mit den verschiedenen Endlagerkomponenten interagieren bei weitem zu komplex ist. Diese Interaktionen sind nicht nur über den gesamten Bereich des Endlagers verteilt, sondern entwickeln sich auch über einen Zeitraum von Jahren und können über einige Tausend Jahre ablaufen. Beeinflusst werden sie durch Faktoren, wie Temperatur, verfügbarer Porenraum sowie Nährstoffkonzentrationen. Um diese verschiedenen Entwicklungen und die Populationsdynamik der Mikroben sowie die Wechselwirkungen mit den Endlagerkomponenten mit einem vertretbaren Aufwand zu beschreiben sollte ein entsprechender Code verwendet werden. Hinsichtlich der Wirtsformation Salz hat GRS bei der Erstellung eines Statusberichts zur Relevanz mikrobieller Prozesse für ein Endlager im Salz, der im Rahmen des Salt Clubs erarbeitet wurde, mitgewirkt. Der Bericht fasst die Rolle von Mikroorganismen in Endlagern in Salzformationen zusammen. Sie basiert auf Informationen zur mikrobiellen Ökologie in hypersalinaren Umgebungen, der Bioenergetik zum Überleben unter Bedingungen hoher Ionenstärken und anderen Studien zu Mikroben in Endlagern. Beiträge der GRS betrafen im Speziellen die Berücksichtigung möglicher Druckeffekte, da die im Endlager erwarteten hohen Drücke Auswirkungen auf die Vitalität und Aktivität von exogenen Mikroorganismen, auf potentielle mikrobielle Metabolismen und auf die Zersetzung von Zellulose haben können.

Ein weiterer wichtiger Aspekt des Projekts war die Betrachtung natürlicher Analoga und ihre Anwendung in einem Safety Case. Eine Aktivität war im Rahmen des Salt Clubs die Organisation eines Workshops, auf dem Studien zu natürlichen und anthropogenen Analoga für ein Endlager in einer Salzformation vorgestellt und hinsichtlich ihrer Verwendung in einem Safety Case diskutiert wurden. Es gab Präsentationen zu vielen Analog-Standorten und -systemen aus verschiedenen Ländern. Die Diskussionsthemen bezogen sich auf Aspekte, die speziell für das Sicherheitskonzept für Endlager im Salz von Bedeutung sind: (1) die Langzeit-Integrität der Steinsalzformation, (2) die Integrität der technischen Barrieren und (3) mikrobielle, chemische und Transport-Prozesse. Ein großer Bereich natürlicher Systeme wurde als potentielles Analogon für die Integrität von Steinsalz diskutiert. Dazu gehörten die Deformation von Anhydritschichten in Steinsalz, die Reaktion von Steinsalz auf mechanische und thermische Belastungen, isotopische Signaturen von syngenetischen Wässern in Fluideinschlüssen. Einige anthropogene Beispiele aus der Öl- und Gasindustrie und aus der Endlagerung chemisch toxischer Abfälle wurden hinsichtlich der Integrität (geo)technischer Barrieren diskutiert. Studien in natürlichen und anthropogenen Salzlaugensystemen wurden als potentielle Analoga für die Radionuklidsorption und -mitfällung, die im Endlager-Nah- oder Fernbereich auftreten können, sowie zur Relevanz von Kohlenwasserstoffen und mikrobiellen Prozessen im Salz identifiziert. Die Diskussionen auf dem Workshop zeigten, dass zu einzelnen, spezifischen Themen, Analoga Studien einen substantiellen Beitrag liefern könnten. Dazu gehören die Kompaktion von Salzgrus-Versatz, die Viabilität von Mikroben im Endlagernahbereich, die Stabilität von Verschlüssen und Isotopen-Signaturen in Fluideinschlüssen.

Ein weiteres Thema war nach Abschluss der umfangreichen Untersuchungen am Standort Ruprechtov in Tschechien die Nachbereitung dieser Analoga-Studie. Der daraus resultierende Statusbericht gibt einen kurzen Überblick über die unterschiedlichen Rollen in nationalen Endlagerprogrammen und ihre Verwendung im Safety Case. Im Bericht werden die Entscheidungen zur Auswahl des Standorts dargestellt, der Standort entsprechend der unterschiedlichen Uran-Lagerstättentypen klassifiziert und die einzelnen Schritte und Entscheidungen während der jeweiligen Projektphase sowie das sich entwickelnde Verständnis über den Standort beschrieben. Vor und Nachteile dieser iterativen Vorgehensweise werden diskutiert. Außerdem beschreibt der Bericht die Erfahrungen die speziell in der Auswahl und Anwendung der experimentellen Labor- und Feldmethoden gemacht wurden und skizziert, wie diese Methoden zu Charakterisierung und Verständnis der Merkmale, Eigenschaften und Prozesse an dem Standort beigetragen haben. Schließlich werden die wesentlichen Erkenntnisse, die relevant für einen Safety Case sind illustriert und die wichtigsten positiven und negativen Erfahrungen bei Standortcharakterisierung und Interpretation aufgezeigt.

Schließlich wurden in einer weiteren Arbeit vorhandene Analoga-Studien für Endlager in Tonformationen zusammengestellt und systematisch analysiert, wie diese Studien einen Safety Case für ein deutsches Endlager in Ton unterstützen können. Als Basis wurde das Endlagerkonzept und die Nachweisstrategie für ein Endlager für wärmeerzeugende radioaktive Abfälle, das im Forschungsvorhaben ANSICHT (FKZ 02E11061) entwickelt wurde, zugrunde gelegt. Entsprechend dem Sicherheitskonzept wird der Einschluss der radioaktiven Abfälle primär durch die Behinderung des Radionuklidtransports aufgrund chemischer und physikalischer Prozesse, die von den positiven Eigenschaften des Tons herrühren, in Kombination mit geotechnischen Barrieren bewirkt. Dieses primäre Sicherheitsziel soll durch weitere untergeordnete Ziele, die im Sicherheitskonzept aufgeführt sind, erreicht werden. Eine Auswahl von existierenden Analoga-Studien wurde dann hinsichtlich ihres Beitrages zu einem oder mehreren Sicherheitszielen begutachtet. Um hinsichtlich der Prozesse und Materialien, die in einem Tonendlager auftreten, möglichst umfassend zu sein, wurde in einem weiteren Schritt überprüft, inwieweit die jeweilige Analoga-Studie zu einem der FEP beiträgt, die im Rahmen der Entwicklung des FEP-Katalogs für ein Endlager im Ton ebenfalls im Vorhaben ANSISCHT zusammengestellt wurden. Die Arbeit zeigt, dass für einige FEP zahlreiche Studien existieren, für manche FEP bisher allerdings keine Analoga vorhanden sind. Basierend auf dieser Auswertung sollten weitere Analoga-Studien einbezogen werden, insbesondere um zu prüfen ob für diejenigen FEP, für die bisher keine Analoga existieren, Analoga gefunden werden können.

Ein Aspekt, der bei dem Prozess der Bentonit-Aufsättigung bisher nicht im Fokus der Betrachtung stand, ist ein möglicherweise begrenzter Wasserzufluss, da unter Endlagerbedingungen der Zufluss aus der Wirtsformation sehr gering sein kann. Bisher wurden Bentonite-Aufsättigungsexperimente üblicherweise mit unbegrenztem Wasserzutritt durchgeführt. Im Rahmen des Vorhabens wurde ein Versuchsaufbau entwickelt und optimiert, bei dem Raten für den Wasserzufluss zu den Bentonitproben so eingestellt wurden, dass sie unterhalb der Aufnahmerate des Bentonits lagen. Damit konnten zeitabhängige Daten zur Wasseraufnahme unter begrenztem Zutritt erhalten werden. Der Rechencode VIPER wurde entsprechend weiterentwickelt, um den begrenzten Wasserzutritt simulieren zu können. Mit diesem erweiterten Modell konnten die experimentellen Ergebnisse zufriedenstellend beschrieben werden. Eine wesentliche Beobachtung aus den Experimenten ist, dass sich eine vollständig gesättigte Bentonitzone, die sich bei Experimenten mit unbegrenztem Wasserzutritt immer im Grenzbereich zum Wassereinstrom einstellt, zu frühen Zeitpunkten der Experimente nicht beobachtet wird, sondern erst zu späteren Zeitpunkten ausbildet.

Vorwort

Der Nachweis der Langzeitsicherheit eines Endlagers für radioaktive oder chemisch toxische Abfälle und damit die Erstellung eines Safety Case erfordert ein umfangreiches Systemverständnis und eine kontinuierliche Verfolgung der Methoden eines Safety Case sowie geeignete und qualifizierte numerische Codes. Das Ziel des Projekts „Wissenschaftliche Grundlagen zum Nachweis der Langzeitsicherheit von Endlagern“, FKZ 02E11102 war es, nationale und internationale Entwicklungen auf diesem Gebiet zu verfolgen, Forschungsprojekte hinsichtlich des Verständnisses, neuer Modellansätze und Daten auszuwerten und spezifische Untersuchungen durchzuführen, um die Methoden eines Safety Case und der Langzeitsicherheitsanalyse zu verbessern.

Das Projekt wurde vom Deutschen Ministerium für Wirtschaft und Energie (BMWi) gefördert und im Zeitraum vom 1. August 2012 bis 31. März 2018 durchgeführt. Die Ergebnisse der wichtigsten Ergebnisse des Projekts wurden in den folgenden Berichten veröffentlicht:

- GRS-349: Natural Analogue Study Ruprechtov (CZ). An Experience Report.
- GRS-430: Hydraulic Interaction of Engineered and Natural Barriers – Task 8b-8d and 8f of SKB.
- GRS-501: Safety Case of Deep Geological Repositories. Scientific Basis and Current Research Results.
- GRS-502: Natural Analogues for Repositories in Clay Formations.
- GRS-503: Bentonite re-saturation - limited access to water and high temperature gradients.

Außerdem wurden substantielle Beiträge zu den folgenden internationalen Berichten erstellt:

- NEA: Natural Analogues for Safety Cases of Repositories in Rock Salt. Salt Club Workshop Proceedings 5-7 September 2012, Braunschweig, Germany.
- NEA: Communication on the Safety Case for a Deep Geological Repository. Radioactive Waste Management, NEA No. 7336.
- NEA: Preservation of Records, Knowledge and Memory (RK&M) Across Generations: Compiling a Set of Essential Records (SER) for a Radioactive Waste Repository.

Abstract

The assessment of the long-term safety of a repository for radioactive or hazardous waste and therewith the development of a safety case requires a comprehensive system understanding, a continuous development of the methods of a safety case and capable and qualified numerical tools. The objective of the project “Scientific basis for the assessment of the long-term safety of repositories”, identification number 02E11102, was to follow national and international developments in this area, to evaluate research projects, which contribute to knowledge, model approaches and data, and to perform specific investigations to improve the methodologies of the safety case and the long-term safety assessment.

This project, founded by the German Federal Ministry of Economics and Technology (BMWi), was performed in the period from 1st August 2012 to 31st March 2018. The results of the key topics investigated within the project are published in the following reports:

- GRS-349: Natural Analogue Study Ruprechtov (CZ). An Experience Report.
- GRS-430: Hydraulic Interaction of Engineered and Natural Barriers – Task 8b-8d and 8f of SKB.
- GRS-501: Safety Case of Deep Geological Repositories. Scientific Basis and Current Research Results.
- GRS-502: Natural Analogues for Repositories in Clay Formations.
- GRS-503: Bentonite re-saturation - limited access to water and high temperature gradients.

Moreover, substantial contributions were developed for the following international reports:

- NEA: Natural Analogues for Safety Cases of Repositories in Rock Salt. Salt Club Workshop Proceedings 5-7 September 2012, Braunschweig, Germany.
- NEA: Communication on the Safety Case for a Deep Geological Repository. Radioactive Waste Management, NEA No. 7336.
- NEA: Preservation of Records, Knowledge and Memory (RK&M) Across Generations: Compiling a Set of Essential Records (SER) for a Radioactive Waste Repository.

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1 Introduction

Within this project strategies and methods to build a safety case for deep geological repositories are further developed. This includes all different aspects of the safety case, namely the assessment basis, methods and strategies, the scientific fundamentals, long-term safety assessment and additional lines of evidence to be used in a safety case. In the international framework the methodology of the safety case is frequently applied and continuously improved. According to definitions from IAEA and NEA the safety case is a compilation of arguments and facts, which de-scribe, quantify and support the safety and the degree of confidence in the safety of the geological repository. The safety of the geological repository should be demonstrated by the safety case. The safety case is the basis for essential decisions during a repository programme. It comprises the results of safety assessments in combination with additional information like multiple lines of evidence and a discussion of robustness and quality of the repository, its design and the quality of all safety assessments including the basic assumptions.

A key element of the safety case is the safety assessment, which represents the evaluation of the performance of a disposal system and the quantification of its potential radiological impact on human health and the environment. The assessment has to demonstrate whether the disposal facility complies with the national regulatory requirements. It is accompanied by an open and adequate addressment of uncertainties. Usually, a comprehensive approach for the handling of the uncertainties is applied including the analysis of the potential evolutions of the repository system and a uncertainty and sensitivity analysis reflecting the uncertainty of model parameters describing the complex repository system. In addition to the quantitative assessment of the repository evolution other arguments are used to support the safety case. One group of arguments are natural analogues, namely processes and features observed in nature with similarity to the processes and conditions expected in the future evolution of the repository system.

The R&D work performed within this project will contribute to the improvement of process and system understanding as well as to the further development of methods and strategies applied in the safety case. Emphasis was put on the following aspects:

- According to international best practice, the development of scenarios for performance assessments of deep geological repositories is based on FEP catalogues. In cooperation with the members of the salt club an international FEP database for repositories in salt, which include information of all available FEP catalogues and available to the public was developed.

- With respect to scenarios, one important question discussed in the German Scenario working group were the requirements and assets of a universal scenario selection method that can be applied in the different phases of the site selection process in Germany as well as for different sites, host rocks, and safety and disposal concepts.

- Regarding the treatment of parameter uncertainty, as part of this project a collaboration with groups from USA, Belgium and Finland was initiated to compare the approaches for probabilistic uncertainty and sensitivity analysis and to learn from each other. Several comparison cases, based on the respective national programmes, were selected for investigation.

- The aspect of adequately communicating the safety case to key stakeholders, particularly the wide public is currently receiving raising interest on national and international level. Substantial contributions were developed for the NEA activities “safety case communication with non-technical stakeholders” and to the “Initiative on the Preservation of Records, Knowledge and Memory (RK&M) Across Generations”.

- In international groups, also technical aspects are discussed, and the respective national experiences are exchanged. on the role of geoscientific arguments in the siting process, and on criticality and safeguards in deep geological repositories. Based on a topical session of the NEA Integration Group for the Safety IGSC and evaluation of the outcome European project FORGE a status report of the role of gases in a safety case was compiled in cooperation with NIRAS-ONDRAF.

- Regarding radionuclide mobility, topics related to the radionuclide inventory, to the source term of C-14 and to microbial processes were content of the project. In cooperation with NAGRA a method for deriving the average and nominal maximum radionuclide inventories of vitrified waste produced at La Hague was developed and applied. GRS participated in the CAST project (CArbon-14 Source Term), which aimed to develop understanding of the potential release mechanisms of C-14 from radioactive waste materials. Major work was contributed to abstract the results produced in the experiments to the scale of the repository system and to analyse their impact in terms of long-term safety.

- Natural analogues are one type of additional arguments, which can be used to support the safety case. Three tasks of the project were devoted to analogues. In the frame of the salt club a workshop “Natural Analogues for Safety Cases of Repositories in Rock Salt” was organised and evaluated. After finalisation of the investigations at the Ruprechtov site in Czech Republic a wrap-up and critical evaluation of the natural analogue study has been performed and compiled in a status report. A third task was devoted to the compilation of analogue studies for radioactive waste repositories in clay formations and a systematic analysis, how such studies can support a safety case.
- With regard to bentonite re-saturation an aspect water uptake under a limited water supply rate from the rock, reflecting potential conditions in a repository system, was addressed. Therefore, in this project an experimental set-up was developed and optimized, where water flow rates where adjusted, which are below the uptake rates of the bentonite samples.

2 Safety case and safety assessment

The safety assessment represents the evaluation of the performance of a disposal system and the quantification of its potential radiological impact on human health and the environment. The assessment has to demonstrate whether the disposal facility complies with the national regulatory requirements. It is a major component of the safety case for a disposal facility and should take into account the potential radiological impacts of the facility, both in operation and after closure and further aspects relevant for safety beyond the quantitative assessment of radiation risks /IAEA 12/, for example (Fig. 2.1)

- operational safety,
- proof of subcriticality,
- inadvertent human intrusion, and
- non-radiological protection goals.

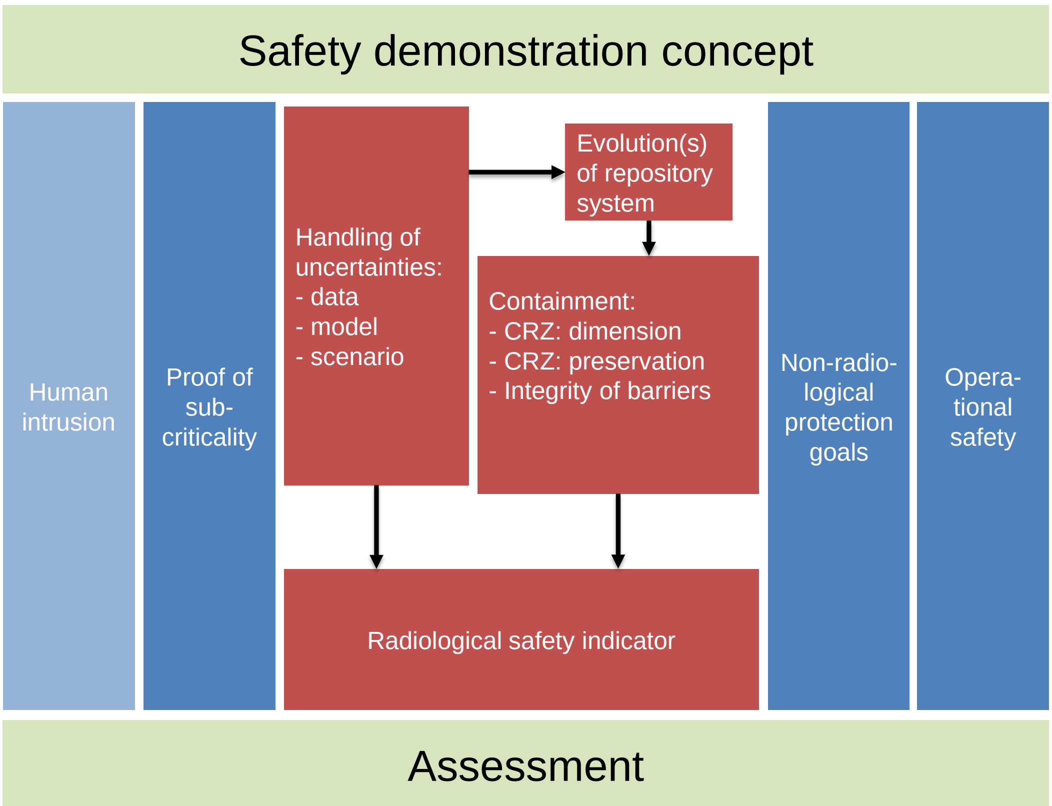


Fig. 2.1 Elements of the safety assessment according to /BOL 17/

The assessment of the post-closure radiological impact forms the core of the safety case for a disposal facility. This involves a comprehensive approach for the handling of the uncertainties, especially the analysis of the evolution of the repository system and the resulting potential radiological consequences. A basic element of the German safety concept is the containment of the radionuclides in a defined rock zone surrounding the mine openings (denoted as containment providing rock zone, CRZ). Isolation will be provided by the depth of the repository and containment by the properties of the CRZ in the long term. For those areas of the CRZ that are penetrated due to the construction of the repository, a technical/geotechnical barrier system must be provided.

Radiological impacts may arise from gradual **Processes** after closure that may cause the facility and its **Features** (e. g. natural and engineered barriers) to degrade (e. g. by corrosion), and from discrete disturbing **Events** that could affect the isolation of the waste (e. g. earthquakes). A systematic approach to describe the evolution of the disposal system is to catalogue all these Features, Events and Processes (FEP) as comprehensively as possible. In the context of a safety case, such a FEP catalogue provides a valuable link between the fundamentals (site description, geoscientific long-term prognosis, and radioactive waste inventory), the repository concept, and the system analysis. In addition to the compilation of the most relevant basics, a FEP catalogue reflects the interrelation between the site-specific conditions and the modifications resulting from the disposal of radioactive waste /LOM 18/. Because of its relevance for the safety case, NEA has implemented a FEP data base, which compiles the international experience of repository projects with different waste inventories and different host rocks. Moreover, the NEA salt club started an activity for developing an international FEP database for repositories in salt, which should include information of all available FEP catalogues and which should be available to the public. This data base should provide future scenario developers with information about relevant processes and effects in all compartments of a repository system including a comprehensive reference data base (Salt Knowledge Archive). The results of these activity are described in detail in Chapter 2.1.

A specific site and the repository system will undergo exactly one evolution, which will be governed both by climatic and geological processes at the site and processes induced by the repository construction and the emplacement of heat-generating waste. Despite a detailed understanding of the various influencing factors, this real evolution cannot be predicted unequivocally in all details. The resulting uncertainty with regard to the future evolution of the repository system can be reduced only marginally by additional research and site investigations. Therefore, a limited number of reasonable possible evolutions are derived in a safety Case based on a systematic assessment of relevant influencing factors with the objective to identify and describe in detail relevant scenarios, which allow to assess post-closure repository safety. The individual scenarios are characterised by FEP that may influence the future evolution of the final repository system. The major activities on the national and international level regarding the development of scenarios are described in Chapter 2.2.

2.1 FEP database for repository in salt

According to international best practice, the development of scenarios for performance assessments of deep geological repositories is based on FEP catalogues /NEA 16/, /BEU 12/. Internationally, many catalogues exist for different host rocks. A survey of FEP catalogues existing about 15 years ago is in the FEP databases of NEA, e. g. /NEA 99/, /NEA 03/, NEA 14/, which comprise complete surveys of FEP names but no detailed descriptions of the FEPs. In Germany, the most recent and comprehensive FEP catalogue for a repository in salt has been developed during the project VSG /WOL 12/. Similarly, in the United States a FEP catalogue for generic deep disposal exists /SAN 13/. These catalogues have been used as a base for the project described in this chapter.

During discussions in the Salt Club (for information to this working group of the NEA-IGSC see /NOS 12/, /NEA 17/) the idea was born to develop an international database for repositories in salt, which should include information of all available FEP catalogues and which should be available to the public. This database should provide future scenario developers with information about relevant processes and effects in all compartments of a repository system. Priority is laid on a systematic, comprehensive and clear list of FEPs to enable users to get a good overview and to check for completeness of FEPs in a future project. Following initial efforts to describe FEPs in many details, it soon became clear, that this work cannot be done within the project, because several hundreds of FEPs would have been to be described.

As a first result an arrangement of the FEPs in a matrix was developed, cf. Fig. 2.2. Any FEP is included in a matrix cell of components (lines) and processes or events (columns). As an example, the FEP “Glass Degradation” is related to “Vitrified HLW” and “Chemical and Thermal-Chemical Processes”. At a workshop in Washington, DC (Feb 1-5, 2016), this matrix was discussed intensively and tested. In the following months, a preliminary comprehensive set of FEPs has been compiled; it actually comprises 448 FEPs.

Characteristics, Processes, and Events / Features / Components		Processes											Events					
	Characteristics	Mechanical and Thermal-M	Hydrological and Thermal-H	Chemical and Thermal-C	Biological and Thermal-B	Transport and Thermal-T	Thermal	Radiological	Long-Term Geologic	Climatic	Human Activities	Other	Nuclear Criticality	Early Failure	Seismic	Igneous	Human Activities	Other
Glossary / Definitions	CP	TM	TH	TC	TB	TT	TL	RA	LG	CL	HP	OP	NC	EF	SM	IG	HE	OE
(GD) General Description	1					1												
Waste and Engineered Features																		
(WF) Waste Form and Cladding	1	5	3	2	2	8	2	3		1					1	2		
(01) SNF and Cladding	1	1		5														
(02) Vitrified HLW	1			2														
(03) Other HLW	1			2														
(04) Metal Parts from Reprocessing	1			2														
(WP) Waste Package and Internals	1	4	8	10	3	9	2	3		1			1	1	1	2	1	
(01) SNF	1																	
(02) Vitrified HLW	1																	

Fig. 2.2 Section of the salt FEP matrix. The numbers in the cells give the number of FEPs related to the corresponding line and column

At the beginning of the project, discussions of FEPs have been based on text files and spreadsheets. It turned out to be more practicable to use an internet-based structure and a webpage has been designed. The webpage has been developed in Germany by a contractor within the project. The first version was released in 2016; a revised version will be available at the end of 2017. Read access to the database is by everybody after registration. Write access is limited to editors. The homepage of the project is now located at http://www.saltFEP.org.

The saltFEP database is under permanent development, but changes cannot be tracked properly at the moment. Thus, a version management is in development and will be available with the next release. It is foreseen to fix the present version, which already includes most FEPs of the VSG and the UFD projects. The aim is to further complete the FEP list, to fix the matrix structure, and to fill out the FEP descriptions to that extent, that the database can be used by the public. Future work will then be to complete the FEP descriptions, which involves descriptions of all occurring processes and events.

2.1.1 Webpage, salt knowledge archive and database

The FEP database is organized electronically as part of the webpage www.saltfep.org. The webpage consists of two parts: the FEP database and the salt knowledge archive, cf. Fig. 2.3. At present, the FEP database is the major part, the salt knowledge archive just being used as a pool of references (see Chapter 2.1.4) for FEP descriptions.

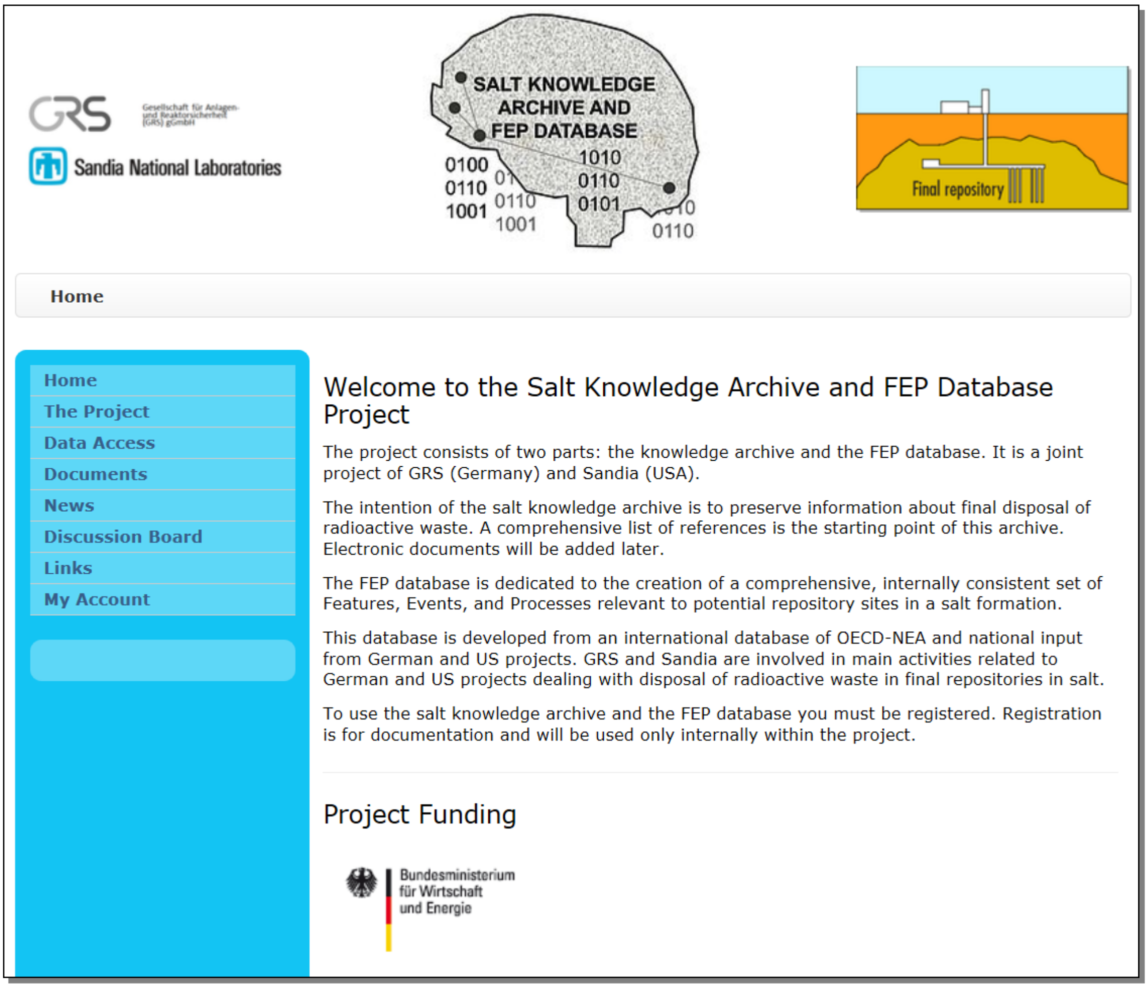


Fig. 2.3 Homepage of saltfep.org

The salt knowledge archive is intended to be a compilation of all available literature in the context of repositories in salt formations. In a first step it shall comprise only references, in a second step related documents (text files, spreadsheets, etc.). Due to copyright requirements, access to the documents will be restricted. The first step is realized in a draft version, i. e. some 900 references of U.S. and German repository projects have been included. Further development of the salt knowledge archive is in progress and will be reported elsewhere.

The actual set of FEPs has been entered into the database. At present, this total set is only accessible to the editors, about half of the set is released to normal users. Access is restricted to those FEPs which have not been reviewed yet or which exhibit preliminary text from former FEP lists not fully adapted to the matrix based FEPs. The content of the FEP database is not yet complete; for most of the FEPs only identifier, FEP description, and associated processes are given. The description of the associated processes, the screening and screening justification as well as the reference lists are still missing for many FEPs.

The menu *data access* in the homepage (Fig. 2.3) is accessible for registered users, all other menu entries are public. At present, focus of the development is on data compilation; minor input is for the other entries.

The SaltFEP database, while fully populated with the set of FEPs and Associated Processes, requires future work to complete the full desired functionality.

2.1.2 FEP list

The main menu of the webpage is shown in Fig. 2.4. In the category *Data Access* all entry points related to FEPs and References are available. As an example, the entry point for the FEP list is indicated by a circle. The FEP list allows write access to new or existing FEPs and read access in two kinds of tables.

Fig. 2.5 shows the List of FEPs in a general view and in Fig. 2.6 in a view with a listing of associated processes and related FEP numbers. By clicking on the pdf-button in the FEP list (right column in Fig. 2.5) the content of the FEP entry is written into a pdf file. By clicking on the edit-button the entry mask for editing is opened, cf. Fig. 2.7. Associated processes are given as rows in the description-decision-justification table, see Fig. 2.8. The screening decision and justification are included in this table, too.

Fig. 2.4 Main menu of the webpage

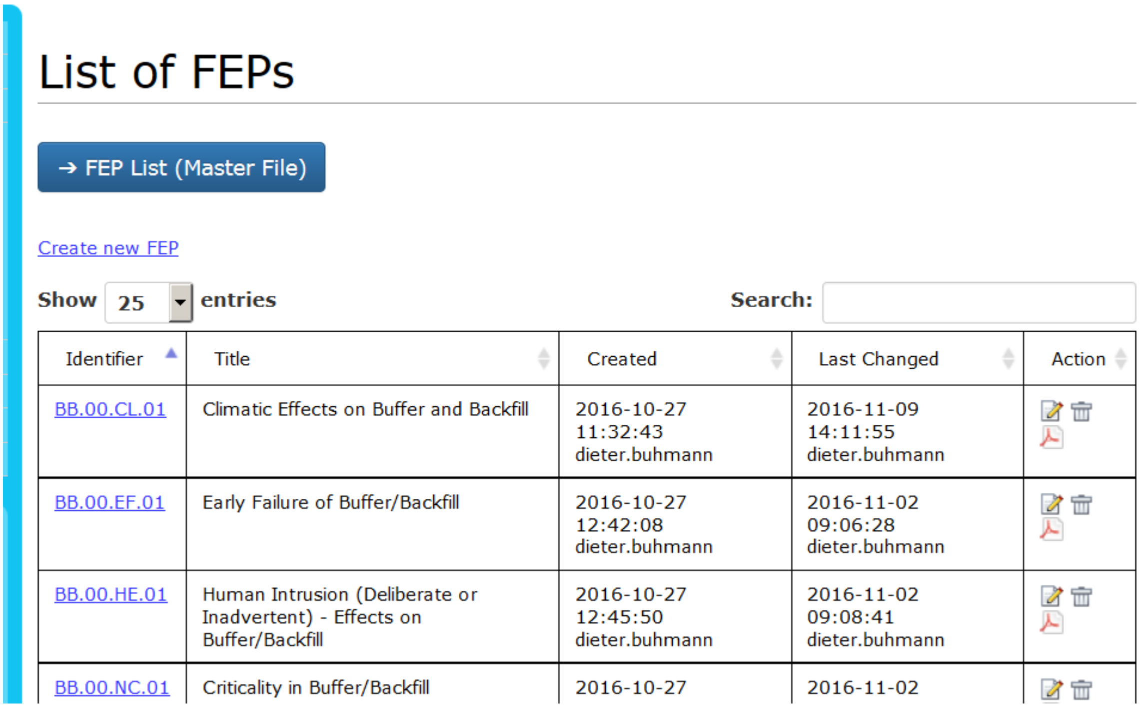
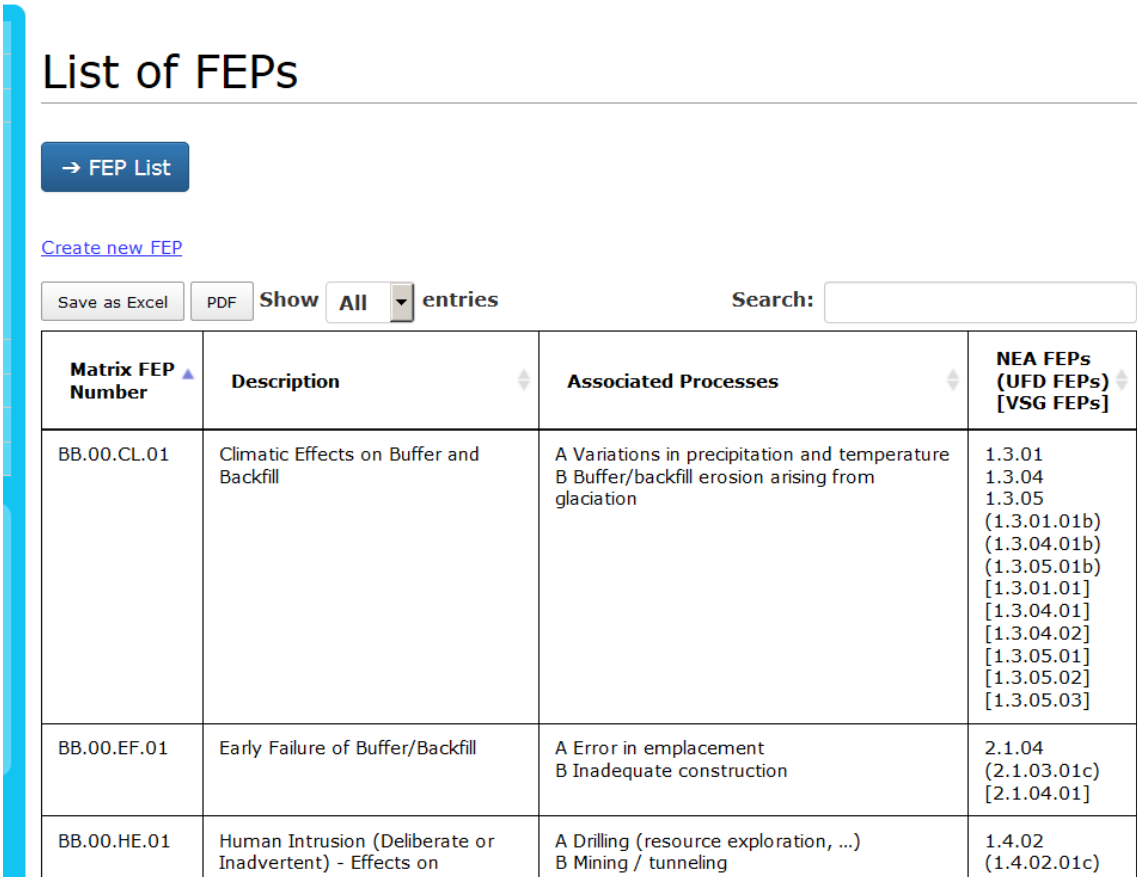


Fig. 2.5 List of FEPs (general view)



List of FEPs

→ FEP List

Create new FEP

Save as Excel | PDF | Show All entries | Search:

Matrix FEP Number	Description	Associated Processes	NEA FEPs (UFD FEPs) [VSG FEPs]
BB.00.CL.01	Climatic Effects on Buffer and Backfill	A Variations in precipitation and temperature B Buffer/backfill erosion arising from glaciation	1.3.01 1.3.04 1.3.05 (1.3.01.01b) (1.3.04.01b) (1.3.05.01b) [1.3.01.01] [1.3.04.01] [1.3.04.02] [1.3.05.01] [1.3.05.02] [1.3.05.03]
BB.00.EF.01	Early Failure of Buffer/Backfill	A Error in emplacement B Inadequate construction	2.1.04 (2.1.03.01c) [2.1.04.01]
BB.00.HE.01	Human Intrusion (Deliberate or Inadvertent) - Effects on	A Drilling (resource exploration, ...) B Mining / tunneling	1.4.02 (1.4.02.01c)

Fig. 2.6 List of FEPs (Master File)

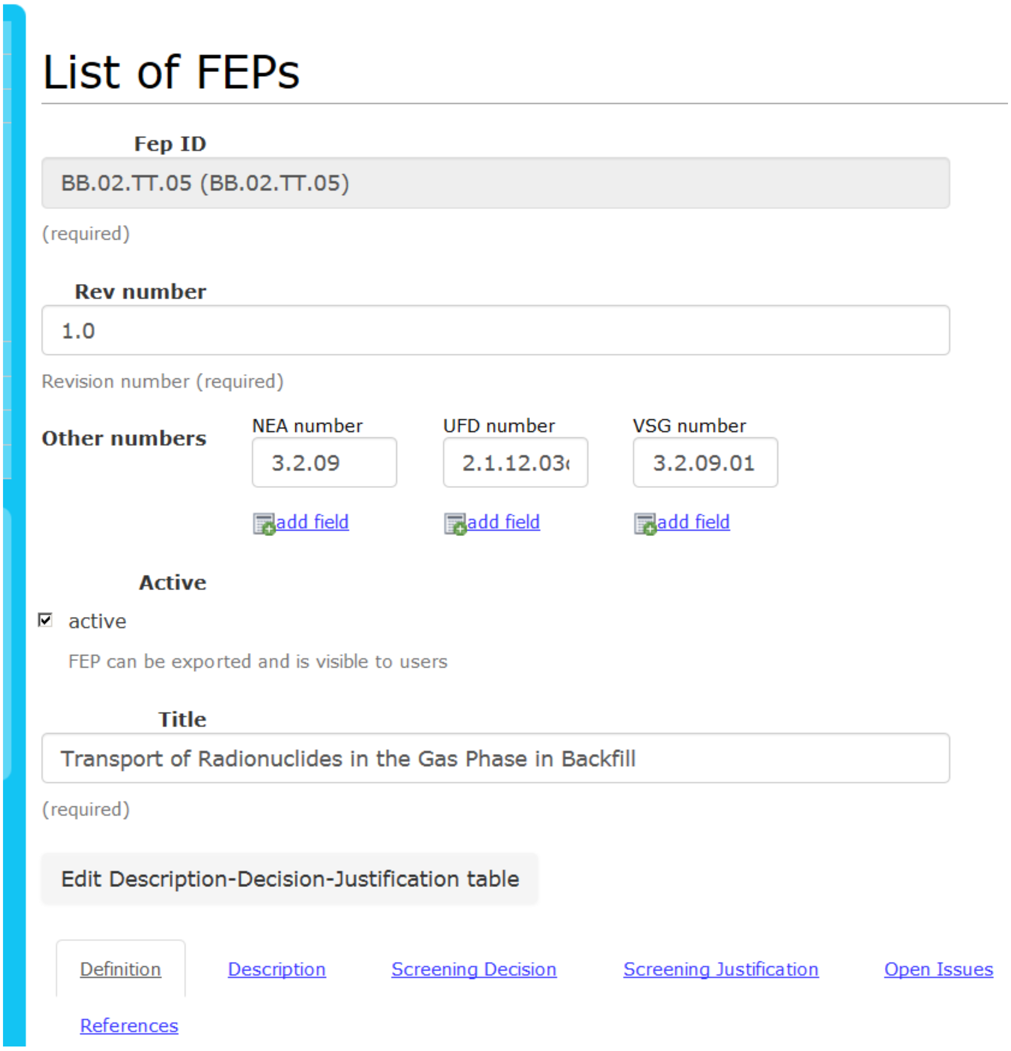


Fig. 2.7 Input mask for FEP description

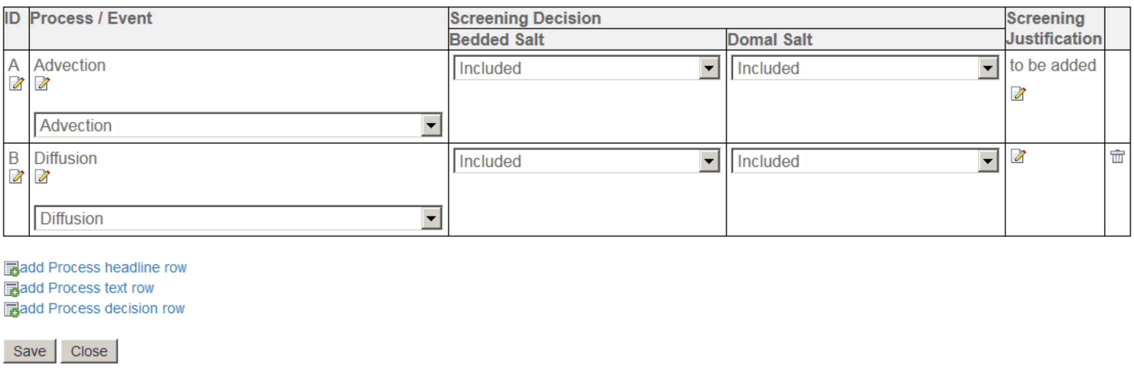


Fig. 2.8 Description-decision-justification table

2.1.3 Further representations of FEP listing

The output of FEPs in the webpage is in different representations. The FEP list described before is the only representation which can be used for editing. At present the following output is implemented for read access:

2.1.3.1 FEP matrix

The FEP Matrix is already mentioned in the introduction of Chapter 2.1. Fig. 2.9 is the actual view of the matrix populated with all the FEPs identified so far. The number in any matrix cell gives the number of FEPs related to this feature/component (row) and process/event (column). If a number is clicked on, these FEPs (or this FEP) are selected and displayed in the *List of FEPs* view, cf. Fig. 2.5 in Chapter 2.1.2.

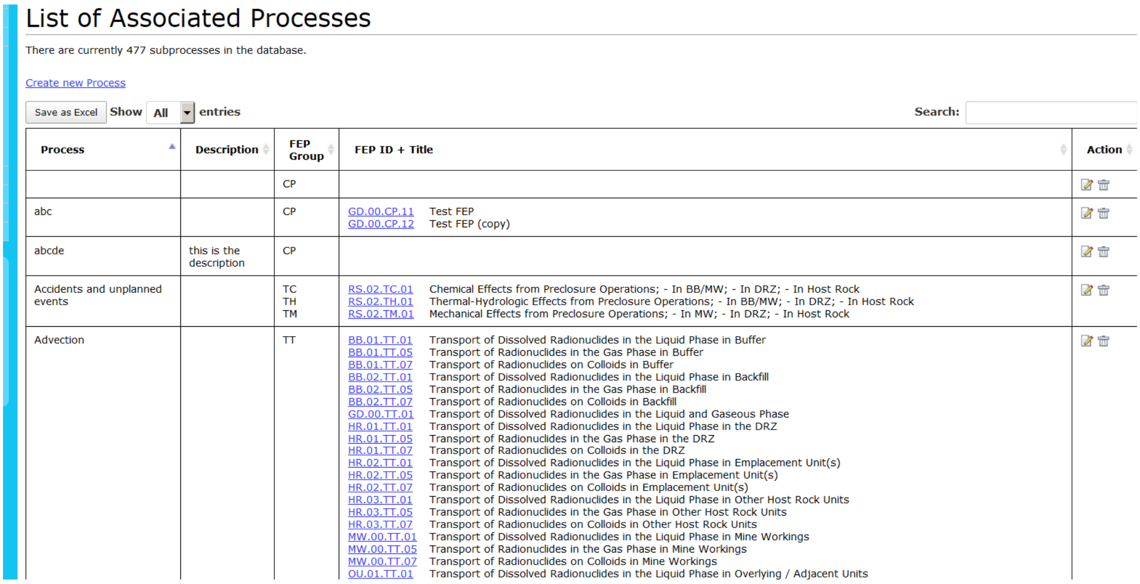
FEP Matrix

Characteristics, Processes, and Events / Features / Components		Processes											Events					
	Characteristics	Mechanical and Thermal-M	Hydrological and Thermal-H	Chemical and Thermal-C	Biological and Thermal-B	Transport and Thermal-T	Thermal	Radiological	Long-Term Geologic	Climatic	Human Activities	Other	Nuclear Criticality	Early Failure	Seismic	Igneous	Human Activities	Other
Glossary / Definitions	CP	TM	TH	TC	TB	TT	TL	RA	LG	CL	HP	OP	NC	EF	SM	IG	HE	OE
(GD) General Description	1					1												
Waste and Engineered Features																		
(WF) Waste Form and Cladding	1	5	3	2	2	8	2	3		1					1	2		
(01) SNF and Cladding	1	1		5														
(02) Vitrified HLW	1			2														
(03) Other HLW	1			2														
(04) Metal Parts from Reprocessing	1			2														
(WP) Waste Package and Internals	1	4	8	10	3	9	2	3		1			1	1	1	2	1	
(01) SNF	1																	
(02) Vitrified HLW	1																	
(03) Other HLW	1																	
(04) Metal Parts	1																	
(BB) Buffer/Backfill							2	3		1			1	1			1	
(01) Waste Package Buffer	1	3	7	2	2	8									1	2		
(02) Drift/Tunnel Backfill	1	3	7	2	2	8									1	2		
(MW) Mine Workings	1	4	7	4	2	8	2	3		1			1	1	1	2	1	
(01) Drift/Tunnel/Room Supports																		
(02) Liners																		
(03) Open Excavations/Gaps																		
(SP) Seals/Plugs	1	3	7		2	8	1	2					1	1	1	2	1	
(01) Drift/Tunnel Seals	1			2						1								
(02) Shaft Seals	1			2						2								
(03) Borehole Plugs	1			2						1								
Geosphere Features																		
(HR) Host Rock	1		1	1	2				6	2			1		1	1	1	
(01) Disturbed Rock Zone (DRZ)	1	4	7	2		8									1	2		
(02) Emplacement Unit(s)	1	4	7	2		8									1	2		
(03) Other Host Rock Units	1	4	7	2		8									1	2		
(OU) Other Geologic Units	1		1	1					6		1		1		1	1	1	
(01) Overlying / Adjacent Units (including Caprock, Aquifers)	1	4	9	2	2	8				2					1	2		
(02) Underlying Units	1	4	7	2	2					1					1	2		
Surface Features																		
(BP) Biosphere					1		1	1		3	1	1			1	1		
(01) Surface and Near-Surface Media and Materials	3	2	3	1		4		2			2	2						
(02) Flora and Fauna	1	1																
(03) Humans	3											2						
(04) Food and Drinking Water								1				1						
System Features																		
(RS) Repository System																		
(01) Assessment Basis	2																	
(02) Preclosure/Operational	3	1	2	1														
(03) Other Global																	1	3

Fig. 2.9 Complete FEP matrix

2.1.3.2 List of associated processes

For any FEP the associated processes are listed in the description-decision-justification table, cf. Chapter 2.1.2 and Fig. 2.8. The *list of associated processes* view compiles all associated processes in the FEP database and gives a link to the FEPs where these processes occur, cf. Fig. 2.10.



List of Associated Processes

There are currently 477 subprocesses in the database.

Create new Process

Save as Excel Show All entries Search:

Process	Description	FEP Group	FEP ID + Title	Action
		CP		
abc		CP	GD.00.CP.11 Test FEP GD.00.CP.12 Test FEP (copy)	
abcde	this is the description	CP		
Accidents and unplanned events		TC TH TM	RS.02.TC.01 Chemical Effects from Preclosure Operations; - In BB/MW; - In DRZ; - In Host Rock RS.02.TH.01 Thermal-Hydrologic Effects from Preclosure Operations; - In BB/MW; - In DRZ; - In Host Rock RS.02.TM.01 Mechanical Effects from Preclosure Operations; - In MW; - In DRZ; - In Host Rock	
Advection		TT	BB.01.TT.01 Transport of Dissolved Radionuclides in the Liquid Phase in Buffer BB.01.TT.05 Transport of Radionuclides in the Gas Phase in Buffer BB.01.TT.07 Transport of Radionuclides on Colloids in Buffer BB.02.TT.01 Transport of Dissolved Radionuclides in the Liquid Phase in Backfill BB.02.TT.05 Transport of Radionuclides in the Gas Phase in Backfill BB.02.TT.07 Transport of Radionuclides on Colloids in Backfill GD.00.TT.01 Transport of Dissolved Radionuclides in the Liquid and Gaseous Phase HR.01.TT.01 Transport of Dissolved Radionuclides in the Liquid Phase in the DRZ HR.01.TT.05 Transport of Radionuclides in the Gas Phase in the DRZ HR.01.TT.07 Transport of Radionuclides on Colloids in the DRZ HR.02.TT.01 Transport of Dissolved Radionuclides in the Liquid Phase in Emplacement Unit(s) HR.02.TT.05 Transport of Radionuclides in the Gas Phase in Emplacement Unit(s) HR.02.TT.07 Transport of Radionuclides on Colloids in Emplacement Unit(s) HR.03.TT.01 Transport of Dissolved Radionuclides in the Liquid Phase in Other Host Rock Units HR.03.TT.05 Transport of Radionuclides in the Gas Phase in Other Host Rock Units HR.03.TT.07 Transport of Radionuclides on Colloids in Other Host Rock Units MW.00.TT.01 Transport of Dissolved Radionuclides in the Liquid Phase in Mine Workings MW.00.TT.05 Transport of Radionuclides in the Gas Phase in Mine Workings MW.00.TT.07 Transport of Radionuclides on Colloids in Mine Workings OU.01.TT.01 Transport of Dissolved Radionuclides in the Liquid Phase in Overlying / Adjacent Units	

Fig. 2.10 List of associated processes

All associated processes can be edited or deleted in this view; new processes can be created and described. The link of an associated process to FEPs is introduced in the FEP list, cf. Chapter 2.1.2.

2.1.3.3 List of decisions

In this FEP catalogue, the screening decision refers to inclusion in, or exclusion from, the PA model. The decisions of the screening process are part of the FEP list and are listed in the description-decision-justification table, cf. Chapter 2.1.2. The *list of decisions* view gives an overview of all decisions (cf. Fig. 2.11) and supports work during the entire screening process.

There are currently 412 FEPs in the list.

Matrix FEP Number	Matrix FEP Name	Associated Process / Event		Screening Decision	
		Process ID	Process Description	Bedded	Domal
BB.00.CL.01	Climatic Effects on Buffer and Backfill	A	Variations in precipitation and temperature	Included	Excluded
		B	Buffer/backfill erosion arising from glaciation	Likely included	Excluded
BB.00.EF.01	Early Failure of Buffer/Backfill	A	Error in emplacement	Included	Likely included
		B	Inadequate construction	Included	Likely included
BB.00.HE.01	Human Intrusion (Deliberate or Inadvertent) - Effects on Buffer/Backfill	A	Drilling (resource exploration, ...)	Included	Excluded
		B	Mining / tunneling	Included	Excluded
		C	Nonintrusive site investigation (airborne, surface-based, ...)	Included	Excluded
BB.00.NC.01	Criticality in Buffer/Backfill	A	Formation of critical configuration	Included	Included
BB.00.RA.01	Radiolysis in Buffer/Backfill	A	He generation from alpha decay in buffer/backfill	Likely included	Likely included
		B	H_2 generation from	Included	Included

Fig. 2.11 List of decisions

In the updated version of the webpage all output tables (representations) will be exportable as spreadsheet and partly as text file (pdf format).

2.1.4 Salt knowledge archive; references

The entry point *References* links to the salt knowledge archive. All information is compiled in a table, see Fig. 2.12. The identifier is unique to a reference and the full description is in a form for usage in citations. The column Remark is a text field for general comments, which are not part of the full description. The column FEPs is the link to the FEP database and described below. In the column Files documents related to the reference can be linked. The documents are stored in a file system on the server parallel to the database.

Show 25 entries Search: hans

Identifier	Full Description	Remark	FEPs	Files	Action
BEC2004a	Bechthold, W., Smailos, E., Heusermann, S., Bollingerfehr, W., Bazargan-Sabet, B., Rothfuchs, T., Kamlot, P., Grupa, J., Olivella, S., and Hansen, F.D. (2004). Backfilling and Sealing of Underground Repositories for Radioactive Waste in Salt (BAMBUS II Project) . EUR 20621 EN, Commission of the European Communities.				
BRO1996	Brodsky, N.S., Hansen, F.D., and Pfeifle, T.W. (1996). "Properties of dynamically compacted crushed WIPP salt" in Proceedings of the 4th International Conference on the Mechanical Behavior of Salt, Montreal, Quebec, Canada, June 17-18, 1996. SAND96-0838C. Albuquerque, NM: Sandia National Laboratories.		BB.02.CP.01 GD.00.CP.11		
CALL99	Callahan, G.D. and Hansen, F.D., 1999. Crushed-Salt Constitutive Model. SAND99-3003C. Sandia National Laboratories, Albuquerque, New Mexico.		BB.02.CP.01		
CAR1980	Carter, N.L. and Hansen, F.D. (1980). Mechanical Behavior of Avery Island Halite, a Preliminary Analysis. ONWI-100, Columbus, OH: Office of Nuclear Waste Isolation.				
CAR1983	Carter, N.L. and Hansen, F.D. (1983). Creep of rocksalt. Tectonophysics , 92(4):275–333.				

Fig. 2.12 List of references

The link to the FEP database acts in two ways: In the column "FEPs" all FEPs are listed which contain the reference. And in the FEP list (cf. Fig. 2.5) for every FEP all references are listed from column 1. As an example: the FEP BB.02.CP.01 (characteristics of backfill) is linked to the references BRO1996 and CALL99 in the table above. Accordingly, these references occur (among others) in the FEP list for the FEP BB.02.CP.01.

Up to now, the database contains no documents (text files, spreadsheets, etc.). This is due to copyright restrictions. It is planned to establish a strict access control for documents in the database. If every user is assigned to the proper access identification, documents will be added and marked by access id. In a first step, access will be only given to internal editors and not to the public.

The establishment of the salt knowledge archive is a long-time project. At this stage, it is just a compilation of references that are widely used in FEP descriptions. In the next steps, further references and finally relevant documents will be added, that cover all fields of knowledge related to final disposal in salt formations.

2.2 Scenario development

Scenario development is an integral part of any safety case. It is used to develop and demonstrate understanding of the system and to show (or to test whether) safety criteria, normally formulated in terms of dose and/or risk, are met for a range of potential evolutions of the disposal system. It is also important for integrating scientific and technical knowledge with a focus on its relevance to the repository safety and thus promoting interdisciplinary communication.

2.2.1 Results from the German scenario working group

The German scenario working group was established in 1997. Its main objectives are:

- establishment of a common understanding with respect to various aspects that are of relevance for scenario development,
- discussion of new international developments and trends, and
- development of joint views and to publish them in position papers.

The permanent members of the working group from Bundesgesellschaft für Endlagerung (BGE), Bundesanstalt für Geowissenschaften und Rohstoffe (BGR), Forschungszentrum Karlsruhe (FZK), Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH, and Technical University Clausthal (TUC), represent those German institutions which pool the respective expertise in scenario development.

Topics that the Working Group has dealt with in the past include

- the definitions of terms,
- the comparison and assessment of methods,
- the categorisation of scenarios into probability classes, and
- how to deal with future human activities, and especially human intrusion into a repository.

One important question discussed in the past five years were the requirements and assets of a universal method that can be applied in the different phases of the site selection process in Germany according to /BGB 17/ as well as for different sites, host rocks, and safety and disposal concepts for the development of scenarios. To answer this question, a set of requirements were identified which focus on one hand on properties/performance and on the other hand on quality characteristics/quality evaluation of an appropriate method /AKS 16/.

A second important topic was the management of evolutions of the repository system that are improbable according to the classification scheme of the German Safety Requirements /BMU 10/. Improbable scenarios include evolutions with a residual probability of occurrence below 1 %, and these have to be analysed and evaluated. It is consensus of the Working Group that it is reasonable to consider only scenarios that have at least a residual probability of occurrence. Unrealistic with a zero or almost zero probability scenarios should be excluded. Instead it is useful to use "What if scenarios" to test the robustness of the repository system (Fig. 2.13). The outcomes of the discussions of the Working Group on the derivation and management of improbable evolutions will be published in 2018 in a further position paper.

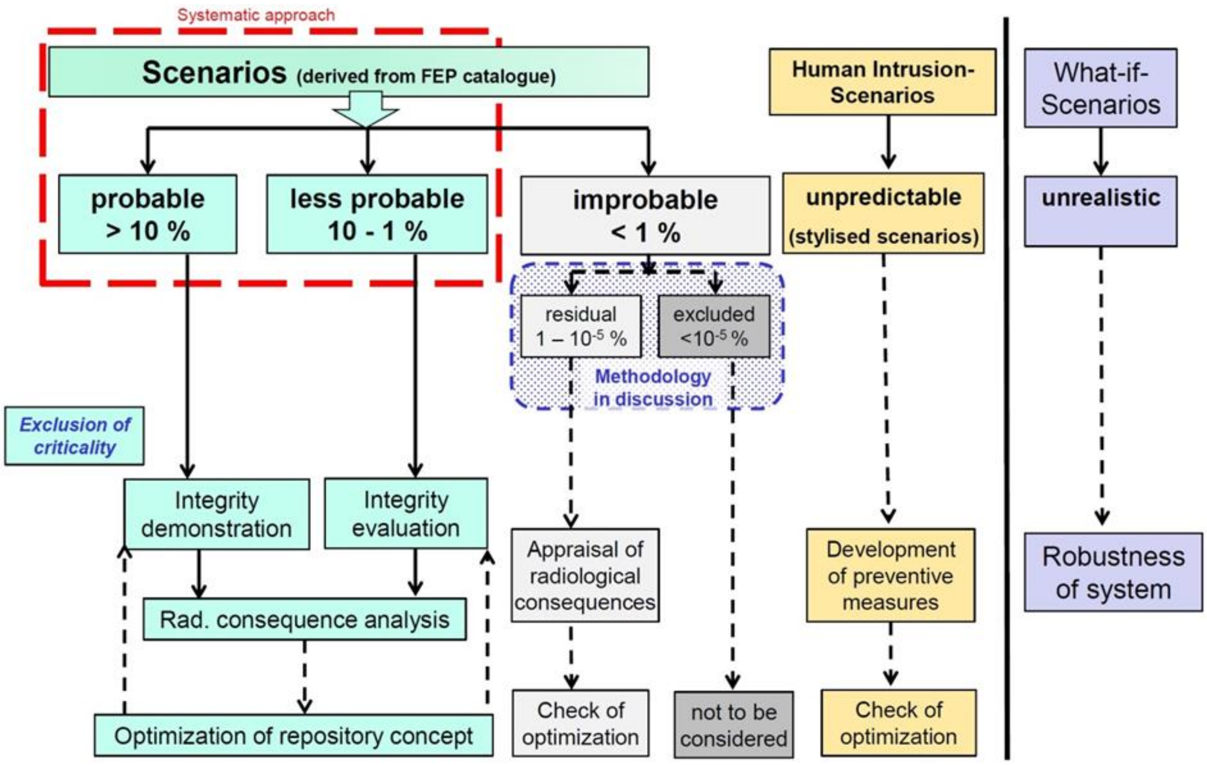


Fig. 2.13 Classification of scenarios and safety demonstration methodology /LOM 18/

2.2.2 NEA

In 1999, the NEA held its first workshop on scenario development in Madrid with the objective to review the methods and application for developing scenarios in a safety case / safety assessments /NEA 01/. Since then, the process of scenario development and analysis for the disposal of radioactive waste has changed and in 2015, the NEA Integration Group for the Safety Case (IGSC) held a second workshop on June 1-3, 2015, in Paris to further evaluate the experience acquired in developing scenarios since 1999. To prepare for this workshop, the IGSC also launched a survey in 2014 to gather the latest scenario development strategies and uncertainty management used in IGSC member countries.

The purposes of the workshop /NEA 16/ were to

- provide a forum to review and discuss methods for scenario development and their contribution to the development of recent safety cases (since the 1999 workshop),
- examine the latest methods and compare their scope, consistency and function within the overall safety assessment process, based on practical experience of applications; and
- provide a basis for producing the present report summarising the current status of scenario methodologies, identifying where sufficient methods exist and any outstanding problem areas.

The outcomes of the workshop are documented in /NEA 16/. The important results are:

1. Since the previous NEA workshop in 1999, work by international organisations, including the NEA MeSA /NEA 12/ and INTESC /NEA 09/ projects, IAEA safety standards /IAEA 12/ and the HIDRA project on human intrusion /IAEA 18/, WENRA safety reference levels /WEN 14/ and the EC PAMINA project /EUR 09/, has provided new insights on scenario development. These insights have been taken up by national programmes in developing and applying scenario development methodologies and in formulating regulations and regulatory guidance. Efforts have been made to ensure comprehensiveness, traceability of decisions, and the integration and logical structuring of interdisciplinary knowledge in the development of scenarios. Scenarios and scenario development also feature more prominently in the documentation of safety cases than was the case in the past, with an emphasis on transparency and traceability of decisions. FEP lists and other tools are used to

confirm that key FEPs and uncertainties are covered adequately in one or more of the identified scenarios and associated calculation cases.

2. In general, scenarios are categorized, based on the types of FEP that are covered in the scenarios, their probability, and their potential effect on the evolution of the repository. In most cases, this classification is determined by regulations or regulatory guidance. For example, in Germany, the safety requirements /BMU 10/ define “probable”, “less probable” and “improbable” evolutions (Fig. 2.13). Terminology used in scenario classification varies widely between national programmes. Irrespective of the differences in terminology, it is possible to distinguish the following generic categories of scenarios:

   – scenarios that aim at representing the foreseeable and expected evolution(s) of the disposal system with respect to the most likely effects of certain or very probable events or phenomena;

   – alternative scenarios that represent less likely but still plausible modes of repository evolutions (e. g. barrier degradation more rapidly than expected) as well as scenarios illustrating extreme natural events (e. g. extreme ice-age or a major seismic event), but that are still within the range of realistic possibilities (bounding cases);

   – what-if scenarios in which implausible or physically impossible assumptions are adopted in order to help bound or conceptually test repository robustness and to assess the relative importance of its various components and safety functions;

   – stylised scenarios, addressing mainly human intrusion and future human actions, which are FEPs for which the probability and consequences are generally considered poorly predictable or unpredictable.

3. The integration of top-down and bottom-up elements may in reality be a feature of all practical approaches to scenario development. Essentially, safety assessors provide a top-down description of the safety concept and safety functions, and “phenomenology” and “technology” provide a bottom-up description of FEP and their attendant uncertainties that could challenge the safety functions, and hence give rise to alternative scenarios. The impact of the perturbing FEP (the initial FEP in the scenario development according to /BEU 12/), either individually or in combination, is then considered when defining scenarios for the evolution of the repository, which are assigned to various categories.

In the proceedings of the workshop /NEA 16/ concluded that clear advances have taken place in recent years addressing key challenges identified in the 1999 workshop. Nonetheless, further development may still be needed, for example in communicating the role and choice of scenarios to wider audiences and on the issue of assigning probabilities to FEP and scenarios.

2.3 Radionuclide mobility

Main work under this topic was dedicated to the European CAST project (CArbon-14 Source Term), which is described in detail below. Beside that a cooperation with NAGRA was performed comparing radionuclide inventories in vitrified high-level waste.

2.3.1 Cooperation with NAGRA

An accurate estimation of the radionuclide inventory of vitrified high-level waste is a prerequisite to assessing the radiological consequences of its geological disposal. The inventories of 34 radionuclides in this waste are provided by the waste producer for individual canisters at the time of loading/delivery. Of these, the inventories of 25 nuclides are measured directly during vitrification and the others are determined by calculation and/or correlation to measured contents.

One purpose of the present work was to cross-check between the average and maximum radionuclide inventories of vitrified waste produced at the same facility in La Hague for Switzerland and Germany based on the data sets reported by the producer for 364 and 3017 canisters, respectively.

Long-term safety assessments of geological repositories require the average and maximum inventories of a further 23 nuclides in addition to the 34 reported ones, which should be estimated by calculation or some correlation based on the technical specifications of the waste and of the reprocessing and vitrification processes. Another purpose of this work was therefore to cross-check these inventories and methods for their estimation as used by NAGRA and GRS.

In particular, the average and maximum nuclide inventories in individual CSD-V canisters assessed by NAGRA and GRS respectively for the Swiss and German glasses were compared. As part of this work, considerable effort was devoted by NAGRA and GRS to determining the radionuclides that are not directly reported by AREVA but are important for safety assessment studies. This estimation was carried out according to the technical specifications given by the waste producer.

The results of the comparison /CAR 15/ show a good agreement for nuclides provided by the waste producer. Fission products such as ^{137}Cs, ^{90}Sr and ^{154}Eu show an agreement within 1 %. The actinides have been found to be within 23 % agreement. The reasons for this deviation can be found in the large fluctuation in the activity value for the actinides, which varies strongly from canister to canister, and in the fact that the compared values are derived by averaging over a very different number of canisters, being 364 in one case and 3017 in the other. The deviations related to the maximum case are really only worse for the $^{239\text{-}241}Pu$ cases (up to 44 %).

The comparison of the nuclides that are not AREVA-declared revealed a number of differences between the inventories, which can be explained on the basis of significant differences in the impurities vector, but not only by this. The largest deviation is observed in the thorium family, especially ^{232}Th, and this is clearly due to the different material definition used by depleting the fuel. In fact, the NAGRA impurity vector ignores the presence of thorium in the fuel matrix, differently from the 5 ppm considered by GRS. Other important differences are observed in the actinides, i. e. ^{226}Ra, ^{227}Ac, ^{231}Pa, ^{232}U and ^{233}U. The build-up of ^{232}U and ^{233}U can be related directly to the alpha decay of the ^{232}Th, which explains the large deviation observed (factor 2.4 and 119 respectively). The other isotopes can be related directly to the depletion and decay of uranium nuclides. Concerning the activation products, there is a good agreement with the exception of ^{59}Ni and ^{63}Ni, due to the higher impurity of nickel employed by NAGRA (seven times more than GRS), and ^{41}Ca, also due to the major content of calcium in the fuel matrix considered by NAGRA (4 times more than GRS). Concerning the fission products, there is a very good agreement for ^{129}I (slightly worse for the maximum case). The NAGRA carry-over fraction for ^{129}I was originally set to 0.0020 /NTB 02/ and has been now increased by more than a factor of 10 in order to agree with the more conservative assumption proposed by the GRS /MEL 12/, /MEL 13/.

Major deviations have been found when comparing the maximum activity glass. The choice of a maximum activity glass has been found to be difficult without fully knowing the effect of various fuel combinations on the parameters of interest, i. e. maximum burnup does not necessarily lead to a maximum activity glass. A very important parameter appears to be the cooling time assumed for the fuel before reprocessing.

For safety assessment studies, the method implemented for deriving the average and nominal maximum radionuclide inventories in glasses is considered to be an acceptable approach. However, for the future it is considered worthwhile to examine a larger variety of glasses to extend this benchmark and to build up a database of possible inventories at an international level; this will allow cross-checks as well as an assessment of the accuracy of the inventory data.

2.3.2 First Nuclides

Integrated performance assessment models of deep geological repositories for high-level radioactive waste (HLW) and spent nuclear fuel include a source term which describes the release of radionuclides from HLW or spent fuel elements (SFE) from failed containers into the contacting aqueous solution. The chemical release rate depends on time (kinetics), solubility of radionuclides in the solution (thermodynamics), and temperature. The general source term can be represented in the form:

$$A_i(t) = n_c(t) \cdot \sum A_{X,i}(t) \cdot r_X \qquad (2.1),$$

where $n_c(t)$ is the fraction of the failed containers at time t, $A_{X.i}(t)$ is the inventory of radionuclide i in component X at time t, and r_X is the chemical release rate for component X. GRS currently utilizes two databases to model the source term with respect to the definition of the components and their characteristic release rates and, correspondingly, the relative inventories of radionuclides in the components.

In the project Scientific Basis for the Assessment of the Long-Term Safety of Repositories, four SFE-components are currently defined: Zircaloy, structural parts, fuel matrix, and instant release fraction (IRF) with the characteristic isotope-independent release rates of 0.0036, 0.002, $1.0 \cdot 10^{-6}$, and 1.0 a^{-1}, respectively. In comparison to the previously used SPA source term with only three SFE components /LÜH 00/ this source term results in significant changes in the calculated effective dose rate. The degree of these changes indicates also a strong dependence on the applied solubility limits, which were assumed for the geochemical environment of a repository, as well as on relative inventories of dose-determining radionuclides ^{36}Cl, ^{129}I, ^{135}Cs, ^{226}Ra, ^{233}U, and ^{237}Np in the components of SFE.

Only three SFE-components were defined in the Preliminary Safety Analysis of Gorleben site: Zircaloy (including tubes and structural materials), fuel matrix, and IRF with the characteristic isotope-independent release rates of 0.00003, 0.00365, and 1.0 a^{-1}, respectively /LAR 13/. The IRF of fission gas, ^{14}C, ^{36}Cl, ^{90}Sr, ^{99}Tc, ^{107}Pd, ^{129}I, ^{135}Cs, and ^{137}Cs is provided for burn-ups of 41, 48, 60, 75 GWd/t_{HM}. Solubility limits in highly-saline brines are provided for Zr, Tc, Sm, Th, U, Np, Pu, and Am and were derived from experimental and analogue studies /KIE 12/. Solubility data for other elements with radionuclides is not available. This is considered presently to be unimportant for performance assessment calculations /LAR 13/. The source term used in performance assessment calculations acts directly on effective dose rate and performance indicators (e. g., radiotoxicity flux from repository compartments) of a repository. These safety and performance indicators can be used to assess the effect of high burn-up fuel on selected scenarios.

GRS committed to contribute to the outcome of the FIRST-Nuclides project by performance assessment calculations for generic repositories for HLW/SF in rock salt and claystone applying an improved source term using parameters for high burn-up SFE provided or derived from data by the beneficiaries of the project. However, because of delays in the progress of the experimental studies of the project and the corresponding lack of new data high burn-up fuel, it was eventually not possible any more to perform these calculations within the time span of the FIRST-Nuclides project.

2.3.3 CAST

The CAST project (CArbon-14 Source Term) aimed to develop understanding of the potential release mechanisms of ^{14}C from radioactive waste materials under conditions relevant to waste packaging and disposal to underground geological disposal facilities. The project focused on the release of ^{14}C as dissolved and gaseous species from irradiated metals (steels, Zircaloys), irradiated graphite and from ion-exchange materials as dissolved and gaseous species.

The objectives of the CAST project were to gain new scientific understanding of the rate of release of ^{14}C from the corrosion of irradiated steels and Zircaloys and from the leaching of ion-exchange resins and irradiated graphite under geological disposal conditions, its speciation and how these relate to ^{14}C inventory and aqueous conditions.

GRS participated in the work package that regrouped the Waste Management Organisations (WMOs) participating to CAST with the aim to consider the results produced in the experimental work packages at the scale of their repository system and to analyse what is their impact in terms of long-term safety. For this issue, the preliminary safety assessment for Gorleben was taken as basis and only Zircaloys and steel were regarded.

2.3.3.1 General outcomes

For the release of ^{14}C from Zircaloy claddings of spent fuel, it has been confirmed in CAST that the source-term of ^{14}C is dominated by the release from the oxide layer and that 1 % of the ^{14}C inventory is a realistic number to account for the very low fraction of accessible ^{14}C that is released. Since the release mechanism is relatively unknown, the validity of the data for the conditions in salt still has to be discussed. Intermediate results indicate that the fraction of organic compounds exceed fraction of inorganic and that the organic speciation might be organic gas. This means that this ^{14}C is in a phase that potentially can be transported in the unsaturated backfill of the repository in salt. The volatile fraction of ^{14}C in the atmosphere of the fuel rod of the assembly is stated to be below 0.2 % according to findings in the First Nuclides project which contradicts previous findings of high fractions of ^{14}C by Smith (1993). This is an issue that has still to be discussed in the future.

For steels a congruent release of ^{14}C with corrosion of the material is assumed. The instant release fraction is assumed to be very low. If the availability of water is limited in the repository in salt host rock, this also could substantially limit the release of ^{14}C. Very low corrosion rates have been determined in CAST that are however not applicable to the situation of a repository in salt due to the differences in temperature and mineralisation of the solution. The statement of congruent release however still could be used as basic assumption with specific corrosion rates for salt derived for non-radioactive material from other projects.

The boundary conditions of the experiments performed in the CAST project do not match the ones expected in the reference evolution of a repository in salt. This is

1.) because of unsaturated conditions prevailing over the time of interest for the release of ^{14}C, while experiments in CAST have been performed under saturated conditions,
2.) because of the fact that those small amounts of fluids existing in the repository show salt concentrations at saturation while the experiments in CAST have been performed with low mineralized waters and

3.) because of the temperatures in a repository concept for high-level waste in salt are likely to be chosen much higher than the 100 °C considered in other types of repository concepts and in the experiments of CAST.

Therefore, the results from the CAST project cannot be directly transferred to the safety case of a repository in salt. Therefore, the simulations performed in CAST used parameter variations to vary the most important influencing factors of the source term and transport of ^{14}C to give first hints about how the source-term of ^{14}C in a repository in salt.

2.3.3.2 Simulations for the ^{14}C release from a HLW repository in salt

2.3.3.2.1 Repository concept

The strategy of the site selection and licensing procedure for a nuclear waste repository for high-level waste in Germany is ongoing at the moment of writing. While salt has been regarded as main option for the host rock for deep geological disposal for some time, the three host rock types salt, clay and crystalline rock are to be considered equally in the future. Although there has been research on repository concepts in clay and crystalline rock, the repository concept for geological disposal in salt host rock clearly is the most advanced at this time. Therefore, the repository concept developed for the Gorleben site within the preliminary safety assessment for Gorleben (VSG) was taken as basis for the work in CAST, has been conducted from July 2010 to March 2013.

The following description of the disposal concept refers to the drift disposal concept developed within the scope of the VSG /BOL 12/ and /BOL 12b/. The emplacement fields for spent fuel and HLW are located in the north-eastern part of the repository. The emplacement fields are tailored in such a way that they are completely embedded in the main salt (z2HS) of the salt dome. The repository layout took into account the known and expected geologic situation at the emplacement level (870 m below surface) of the salt dome. Two main transport drifts are the northern and southern boundaries of the twelve emplacement fields (East 1 to East 12). Each emplacement field consists of a crosscut and several parallel emplacement drifts in which the waste containers are emplaced on the floor. After the containers have been emplaced, the void spaces of the emplacement drifts are backfilled with dry crushed rock salt. There is no requirement to seal each single emplacement drift. Optionally, the emplacement field is sealed with a 10-m-long sorel concrete (MgO) plug at both ends of the crosscuts for operational reasons. Sorel concrete consists of magnesium oxide as adhesive cement and crushed salt as aggregate. These plugs have no specified requirement for the post-operational phase. The main transport drifts are backfilled with crushed salt as well, but with a water content of 0.6%wt, to accelerate the compaction process.

2.3.3.2.2 ^{14}C inventory

The inventory of the repository consists of heat generating waste. Waste types with negligible heat generation which are foreseen to be disposed of in the already licensed repository Konrad are not considered here. The data given was collected in the German research project Preliminary Safety Analysis for Gorleben (VSG). It considers the disposal of the following heat generating waste types:

- Spent fuel elements (SF) for direct disposal from pressure water (DWR), boiling water (SWR), water-water (WWER) and research reactors as uranium oxide (UO2) or mixed oxide (MOX) fuel,
- Vitrified reprocessed spent fuel (CSD-V) mainly from reprocessing in France and Great Britain,
- Vitrified effluents and sludges from reprocessing (CSD-B) and
- Compacted Zircaloy hull material and metal parts from disassembled SF-elements (CSD-C).

The absolute amount of the wastes to be disposed of in the future that fall into these four categories are fairly well known due to the phase out from nuclear energy in Germany. The expected inventories are given in /PEI 12/. The radionuclide inventory of the spent fuel was calculated using the OREST-code assuming a burn-up of 50 GWd/t_{hm} for SWR fuel elements, and 55 GWd/t_{hm} for DWR fuel elements with a potential Nitrogen impurity of 30 ppm. Information on other impurities, the uranium enrichment of the fuel, the chemical composition of the hull material and information on the burn-up calculations, like neutron fluxes are also given in /PEI 12/. The inventory of the CSD-C waste was obtained from the same OREST simulations with assumed Nitrogen impurities in the Zircaloy hull material of 45 ppm /HUM 01/. Nitrogen impurities in the metal parts are not given in the documentation of the calculations. The inventory of the CSD-V type of waste was also received from OREST calculations regarding DWR fuel elements with a burn-up of 33 GWd/t_{hm} and the same values for nitrogen impurities as for the spent-fuel given above. This inventory used in VSG for CSD-V does not correctly take into account the actual distribution of ^{14}C in the different waste streams during the reprocessing at La Hague. This is why the inventory is expected to be by far too high. A more realistic estimation comes to the conclusion that the ^{14}C inventory per CSD-V canister delivered to Germany from La Hague can be estimated to range between the minimum value of 84.6 MBq and the maximum value of 517 MBq with an expected, average value of 238 MBq /MEL 12/.

The type of packaging is not yet decided and depends on the repository concept and host rock type. The drift disposal concept (concept B) of the VSG assumes the use of POLLUX containers which can hold up to 30 SWR fuel elements with 0.177 tons heavy metal (t_{hm}) each or 10 DWR fuel elements with 0.52 t_{hm} each.

As an option, the additional storage of waste types with negligible heat generation in a separate second repository wing with a distance between both wings of about 400 m was examined within the scope of the VSG (concept A). The waste types considered in this option are:

- wastes containing graphite which mainly stem from neutron reflector shields from the high temperature rector (AVR),
- depleted Uranium tails which stem from the production of fuel elements, and
- other, non-specified wastes which are not applicable to be disposed of in the future Konrad repository.

The waste categories listed under items 6 to 7 are on the one hand still ill-defined in terms of waste amount, packaging and chemical form and on the other hand, it is not yet decided whether those types of waste will be deposited in a future repository primarily constructed for heat generating waste at all. Therefore, these waste types are not considered in the following and the data given in Tab. 2.1 only refers to the given list items one to four. The full nuclide vectors of the given waste types and additionally for the spent fuel from six research reactors are also listed in /PEI 12/.

The uncertainty of the ^{14}C inventory of spent fuel and hull material directly results from the uncertainty in the assumptions of the burn-up calculations for spent fuel and additionally from the assumptions concerning the reprocessing process for reprocessed CSD waste types. The assumed Nitrogen impurity of 30 ppm in the spent fuel used for the calculations of the numbers given in table 1 is an upper bound of the expected range. The lower range can be assumed to be 4 ppm resulting in an uncertainty of the resulting ^{14}C inventory of a factor 3.6 /HUM 01/. Impurities of Nitrogen in Zircaloy-4 were assumed to be in the range of 45 to 75 ppm. The numbers in Tab. 2.1 refer to the latter value. No information is given on the bandwidth of the other assumptions used in the burn-up calculations or of the resulting uncertainty of the calculated activities. No information is available on the uncertainties regarding the assumptions for the reprocessing process of the CSD waste types. However, since some uncertainties were already identified in /MEL 12/ regarding the CSD-V waste types the inventories of the other two CSD wastes might also be subject to higher uncertainties. No information is available on the chemical form of the ^{14}C.

Tab. 2.1 Inventory of ^{14}C for the main heat generating waste families stemming from the use of power reactors

Waste type	**Number of fuel elements**	**^{14}C activity [GBq/t_{hm}]**
SF (SWR) UO2	14,350	37.7
SF (SWR) MOX	1,250	21.9
SF (DWR) UO2	12,450	37.3
SF (DWR) MOX	1,530	23.1
SF (WWER) UO2	5,050	10.2
	canisters	[GBq/canister]
CSD-V	3,735	17.9
CSD-B	308	not listed
CSD-C	4,104	13.8

2.3.3.2.3 Reference scenario

The reference scenario is chosen according to the work performed for the preliminary safety assessment for Gorleben (VSG) /LAR 13/. In the reference case, the sealings behave for at least 50 000 years as designed and the porosity of the salt grit backfill in the drifts reduces down to 1 % within a few hundreds to a few thousands of years. The according permeability of the salt grit is estimated to be $k = 3 \cdot 10^{-20}$ m², which is sufficiently low to reduce the inflow along the drifts into the mine to a value that the repository mine is still not fully saturated at the end of the reference period of one million years. No advection, but only diffusive transport is effective for the radionuclides dissolved in the liquid phase for such conditions. No dissolved radionuclides are released from the isolating rock zone during the whole reference period. Consequently, the contribution of dissolved radionuclides to the RGI is zero for the reference scenario.

For the simulations of the gas transport pathway, a lifetime of 500 years is assumed for the waste containers, with the exception of four containers which are assumed to have initial defects already at the time of emplacement. As a conservative assumption, it is assumed that the volatile radionuclides can be instantaneously released from these containers.

For the release of ^{14}C from the spent-fuel containers, the instant release fraction (IRF) of ^{14}C is assumed to be 10 % for the UO_2 fuel matrix, 10 % for the Zircaloy and 20 % for the metal structural parts. For the CSD-C containers from reprocessing, no IRF of ^{14}C was assumed due to the acid treatment of the material which removes the oxide layers. No bandwidths have been assumed for those values. No information is available if those are realistic or rather conservative values.

^{14}C from the IRF in the matrix and in the metal parts is assumed to be released not before a contact of external water with the waste. However, the 10 % of the ^{14}C in the IRF of the Zircaloy disposed with the spent fuel is assumed to be in oxide layers and is assumed to be released instantaneously as CO_2-gas after container failure, even without a contact of the waste matrix with external waters. This assumption is based on /SMI 93/ and subsequent publications and is clearly a conservative assumption.

A flow of non-radioactive gases in the mine is caused from the beginning of the post-closure phase by the displacement of air from the mine. This is due to the convergence of the salt host rock and the decreasing porosity in the salt grit. Additionally, a gas flow also results from hydrogen production caused by iron corrosion by the small amount of water initially emplaced with the containers and the salt grit backfill. External waters that might reach the emplacement fields closest to the shaft can potentially lead to a more significant corrosion and gas production, however to late times which are not relevant for the ^{14}C release.

The ^{14}C instantaneously mobilised from the IRF of the Zircaloy is released from the four initially defect spent fuel containers directly at the beginning of the post-closure phase and further on is transported along with the non-radioactive gases through the unsaturated drifts to be released through the drift seal from the IRZ.

2.3.3.2.4 Simulation model

TOUGH2 was used to model the gas and radionuclide transport in the mine to perform the simulations as part of the CAST project. The modelling with TOUGH2 needs a representation of the repository as a segment structure. The segment structure used for the simulations presented in the following is based on the one used for the simulation of the dissolved radionuclides using the near-field module LOPOS for repositories in salt from the RepoTREND code family /BUH 16/. The structure consists of 46 segments (see Fig. 2.14) representing the full repository layout. The LOPOS segment structure is directly converted into a TOUGH2 segment model. For the TOUGH2 simulations in the project CAST only the spent fuel in Pollux-containers and the compacted hull material in CSD-C containers are regarded. These waste forms are stored in the emplacement areas in the east wing. Therefore, all segments representing the west wing were removed from the segment model (shaded in grey in Fig. 2.14).

The standard version of TOUGH2 regards temporal constant porosity and permeability material parameters. This is not representative for the situation in salt, where the convergence of the backfill leads to a decrease in permeability and porosity and consequently in a gas flow of the air being expelled from the pore space during compaction acting as carrier gas for volatile radionuclides. The latter effect is of most importance for the release of radioactive gases. In the VSG a modified version of the TOUGH2 code has been used that was extended to be capable of considering the convergence process. Since this modified version of the TOUGH2 code is not public available, a different approach has been used in the following to regard the effect of the flow of expelled air acting as carrier gas for the radioactive gases: The convergence of the salt and the resulting reduction of the porosity of the salt grit is simulated by assuming a source of air at a constant low porosity. However, the effect of changing porosity and permeability cannot be regarded by this approach.

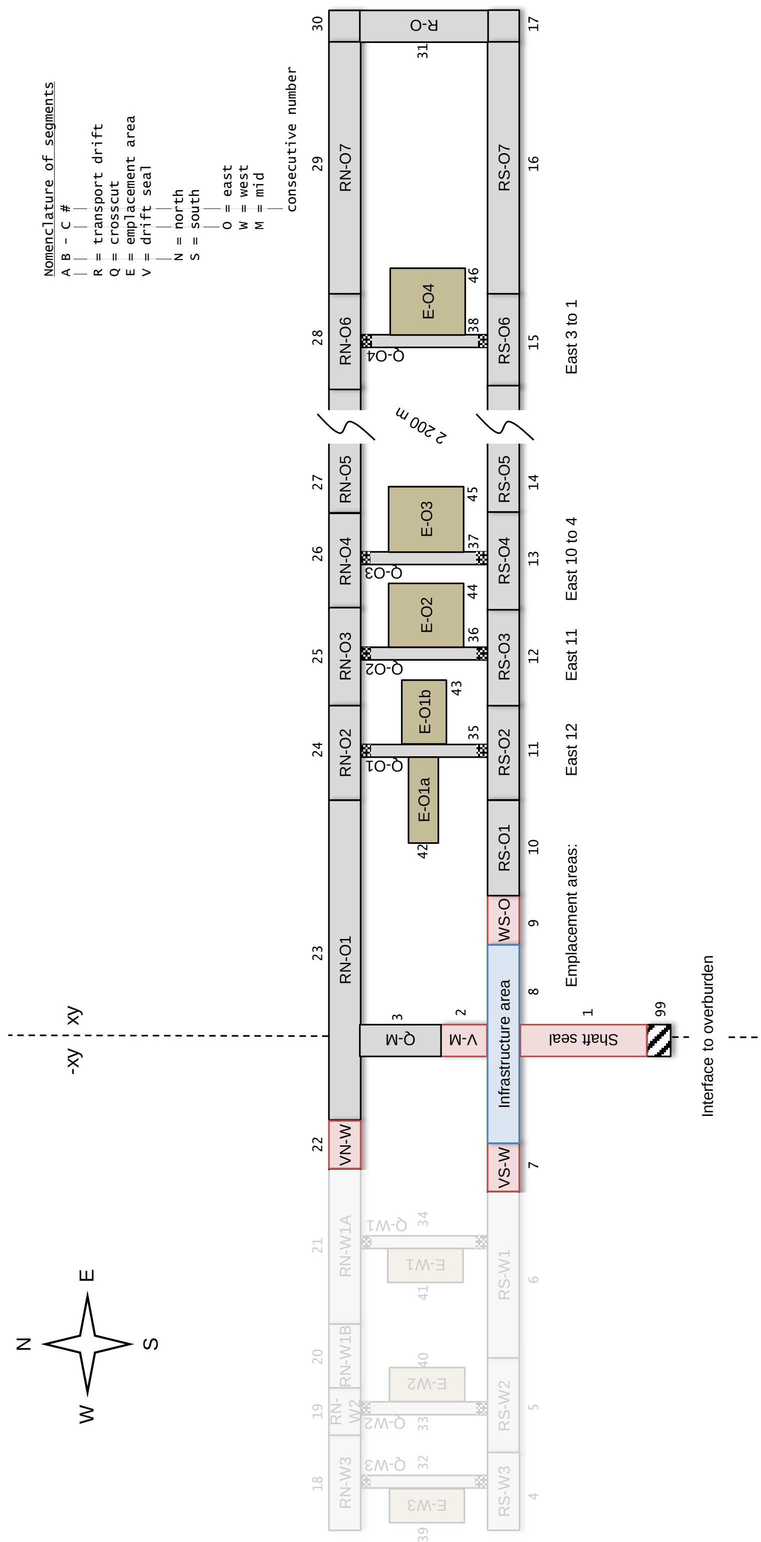


Fig. 2.14 Segment structure of the repository model (not to scale)

The change of porosity of the segments as modelled in the LOPOS model is shown in Fig. 2.15 for three segments. This temporal behaviour is calculated during the simulation and is segment specific due to the different temperature at different locations. For the TOUGH2 simulation, the convergence has been assumed similar for all segments and the pore volume of each segment is reduced by 1/8 of its volume each year, what fits quite well to the behaviour calculated in the LOPOS model. Due to the different initial size of the segments, the resulting gas flow is however different for each segment (see Fig. 2.16). Segment 16 for example has an initial volume of about 23,000 m^3. With an initial porosity of the backfill of 0.35 the initial pore volume is about 8,050 m^3. The porosity is reduced with time by convergence resulting in either an outflow of nearly 8,000 m^3 of air from this segment or in an increase of air pressure. A combination of both happens in reality. After 200 to 300 years, most of the air is generated by the assumed sources and has either been expelled from the mine or lead to an increase of gas pressure using this approach. The convergence finally comes to an end at 500 years. After that point in time further gas flows only occur by either equalling out existing gas pressure differences or by diffusion to equal out concentration gradients.

Since permeability and porosity are constant in TOUGH2, effective mean values have to be assumed for both parameters. Effective (mean) porosity and permeability have not necessarily fit together according to the porosity-permeability-relationship of crushed salt, since both work on different scales and the effective mean value results from different weighing. Constant values have been chosen of 5 % for the porosity and 10^{-15} m^2 for the permeability of the salt grit.

Two initially defect containers are assumed, one in each of the emplacement areas E-O1a and E-O1b. Each of the two containers releases the IRF of ^{14}C of $5.6 \cdot 10^{-9}$ Bq into the air of the emplacement area during one year after time t = 0 resulting in a release rate of $1.08 \cdot 10^{-12}$ kg/s of ^{14}C. Additionally, all other containers in those two emplacement areas, i. e. 10 containers in emplacement area E-O1a and 100 containers in E-O1b have been assumed to fail after 500 years and releasing their IRF of ^{14}C into the gas phase.

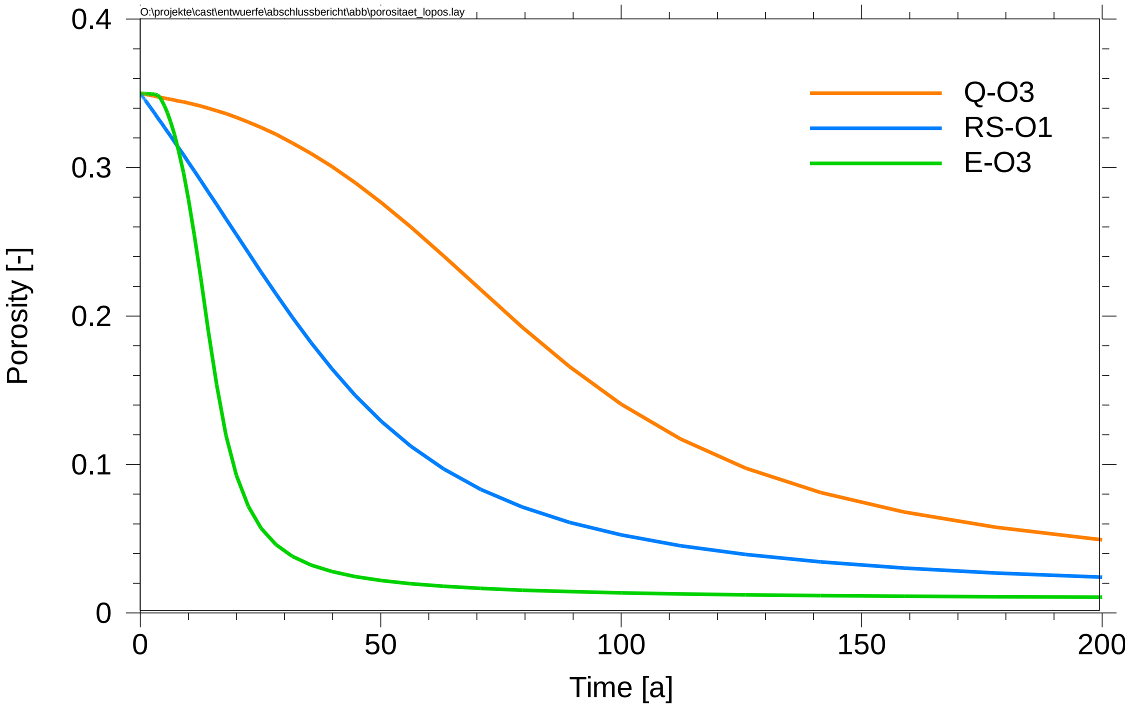


Fig. 2.15 Temporal evolution of three segments in the LOPOS model

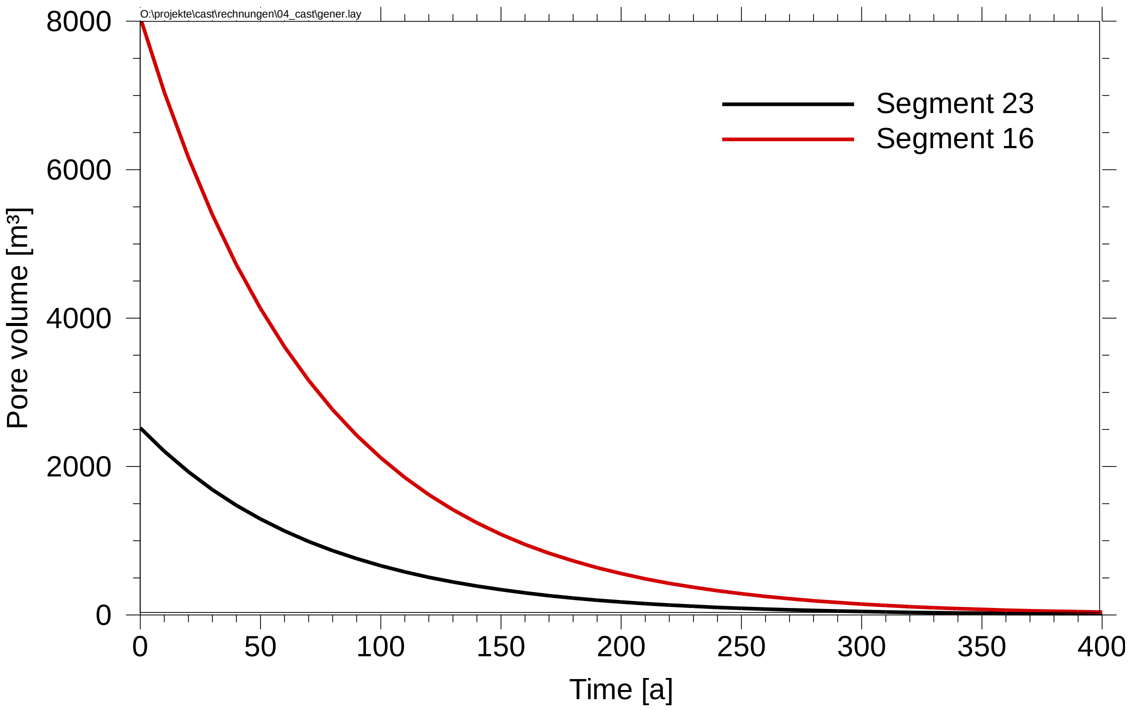


Fig. 2.16 Temporal evolution of pore volume for selected segments

2.3.3.2.5 Results and discussions

The results of the simulations are presented as RGI values and are therefore directly comparable to the results presented in the VSG /LAR 13/. For the model presented, the RGI values are calculated as sum of the ^{14}C fluxes at the drift seals V-M (segment 2) and WS-O (segment 9). Since the standard TOUGH2 code used in the simulations presented here is not able to allow for temporal variable porosity and permeability values, parameter variations have been performed to estimate their influence on the maximum RGI value (see Fig. 2.17 and Fig. 2.18). Tab. 2.2 shows the maximum RGI value depending on the porosity and permeability values given. In principle it can be said that in this model, higher porosity values lead to lower RGI-values and for higher permeability values there is a tendency to obtain a curve with for two peaks. Lower permeability values result in two effects which are that the first peak is moving towards later times and has a lower RGI value. Lower permeability and porosity values also tend to result in higher gas pressures in the mine. The first peak in the RGI-plot may even fall together with second peak, resulting in one single peak. The result of the simulations shows a variation of the RGI of about one to two orders of magnitude for reasonable parameter variations. A permeability of 10^{-15} m^2 and a porosity of 0.05 have been chosen for the further simulations.

The major contribution of the overall RGI is from the flux out of segment WS-O (segment 9) and results from the two initially defect containers. Other containers failing after 500 years only result in a minor relative maximum in the curve after about 83 000 years with an RGI lower than 10^{-7}. The peak of the RGI-plot is much wider than presented in the VSG-simulations /LAR 13/. The reason is most probably that the convergence in the emplacement areas is much faster in the VSG-simulations: the convergence is already finished after some tens of years for the emplacement areas, resulting in a much faster movement of the gases and a much sharper peak of the RGI.

Tab. 2.2 Maximum calculated RGI-value when varying the parameters of the backfill for porosity *n* and permeability *k*

***k* [m²]** / ***n* [-]**	**10^{-14}**	**10^{-15}**	**10^{-16}**
0.02	3.5	2.1	0.9
0.03	0.7	0.4	0.3
0.05	0.1	**0.1**	0.1
0.10	0.02	0.02	0.02

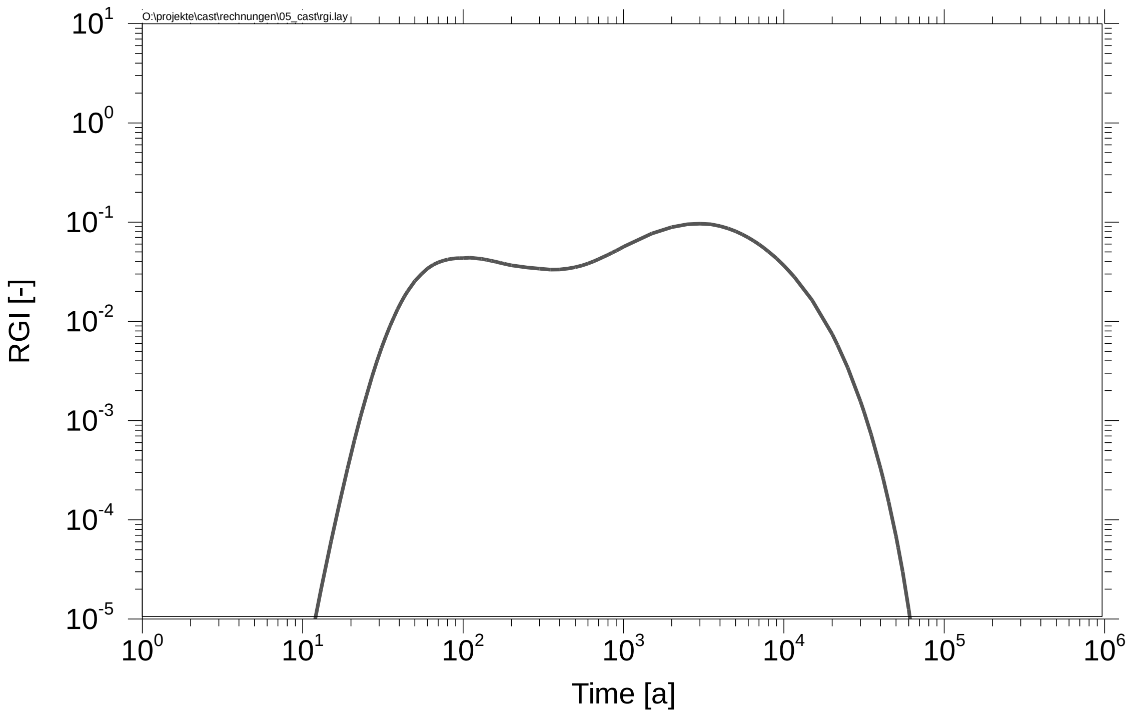


Fig. 2.17 Temporal evolution of the RGI-value for a reference parameter combination for porosity and permeability of $n = 0.05$ and $k = 10^{-15}$ m^2

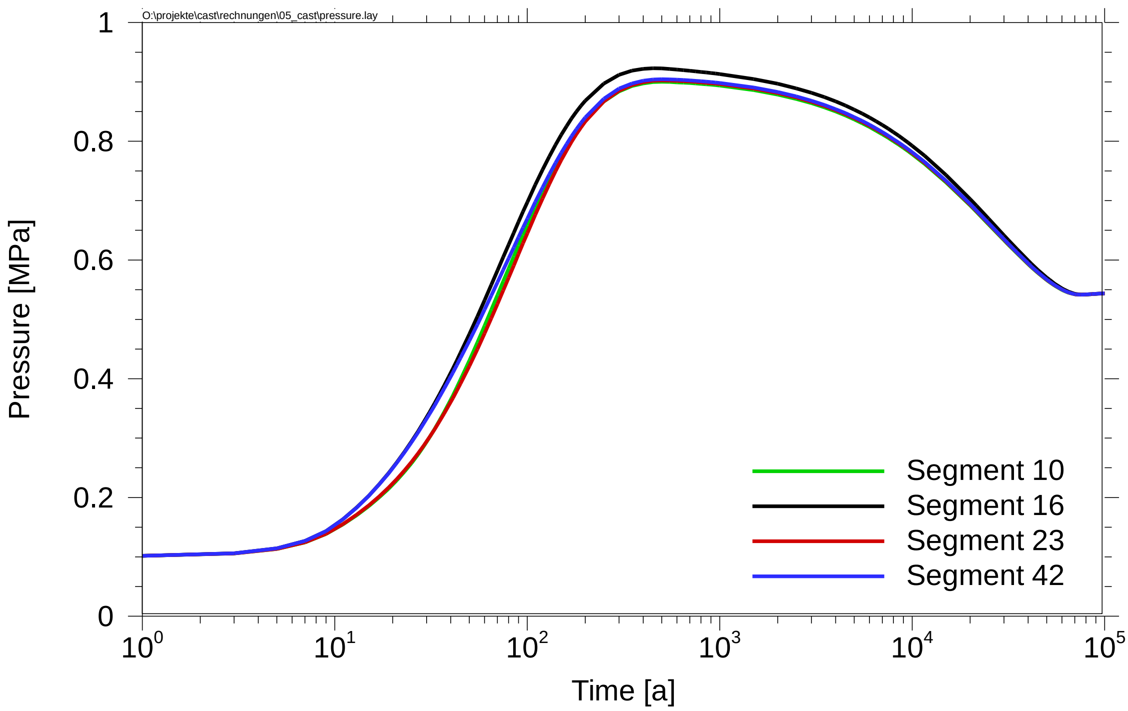


Fig. 2.18 Temporal evolution of pressure for selected segments for a reference parameter combination for porosity and permeability of $n = 0.05$ and $k = 10^{-15}$ m^2

The boundary conditions of the experiments performed in the CAST project do not match the ones expected in the reference evolution of a repository in salt. This is on the one hand because of unsaturated conditions prevailing over the time of interest for the release of ^{14}C and on the other hand because of the fact that those small amounts of fluids existing in the repository show salt concentrations at saturation. Therefore, the results from the CAST project cannot be directly transferred to the safety case. Since the experimental results obtained in CAST are not directly applicable to the situation in salt, parameter variations are performed to vary the following influencing factors of the source term:

Instant release fraction (IRF): The IRF was varied to be 10, 1 and 0.1 percent of the ^{14}C inventory equally for all compartments of the spent fuel waste package.

Release rate: The release rate was varied in a way that the release started at the beginning of the simulation and lasted for 1, 10, 100 and 1000 years respectively.

Release start time: The time of the IRF release start was varied to be 1, 10, 100 and 500 years with a release of the full IRF within 1 year after the release time.

The reference values considered are always the ones given at first in the list above. All other parameters have been used as described before for the reference case. The simulations presented in the following aim to investigate how the variation of the source-term of ^{14}C does affect the outflow of ^{14}C from the repository i. e. the radiotoxicity indicator RGI.

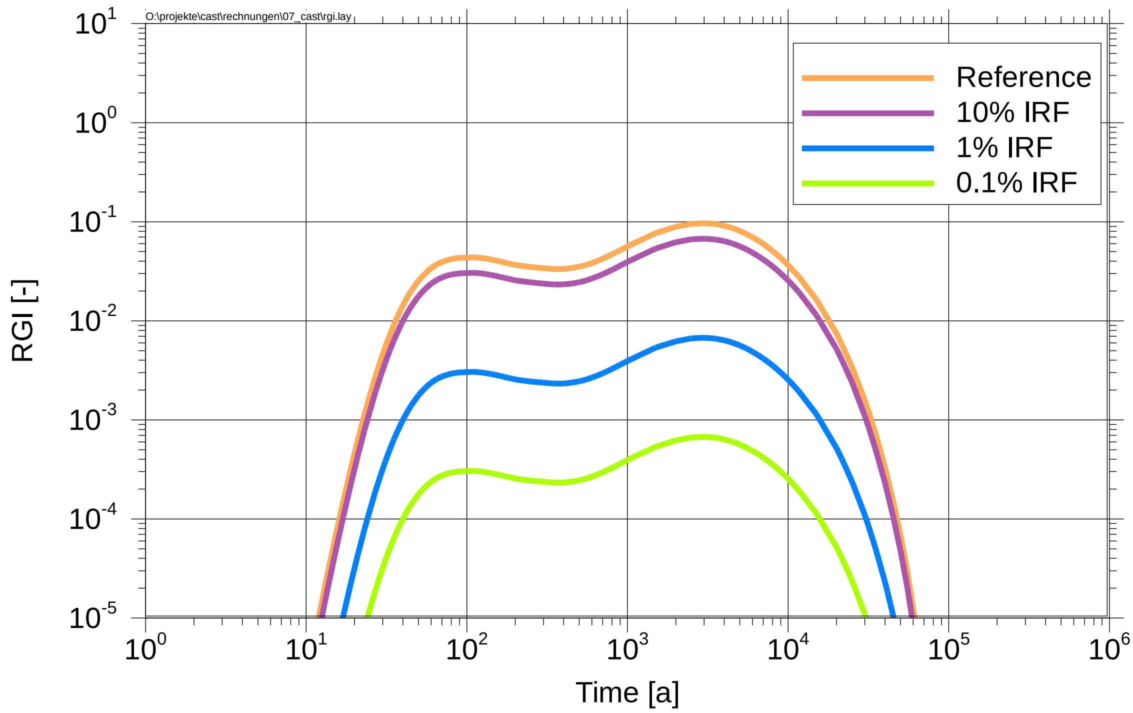


Fig. 2.19 Dependence of the radiotoxicity indicator RGI from the ^{14}C IRF

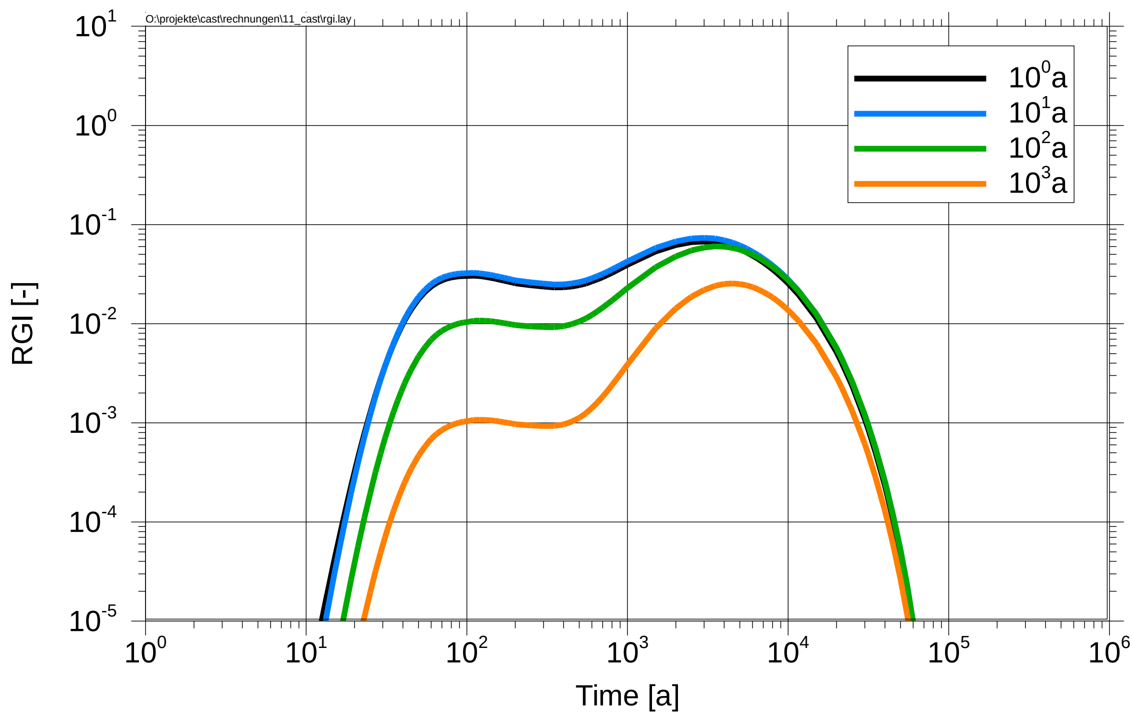


Fig. 2.20 Dependence of the radiotoxicity indicator RGI from the release rate of ^{14}C for an IRF of 10 %

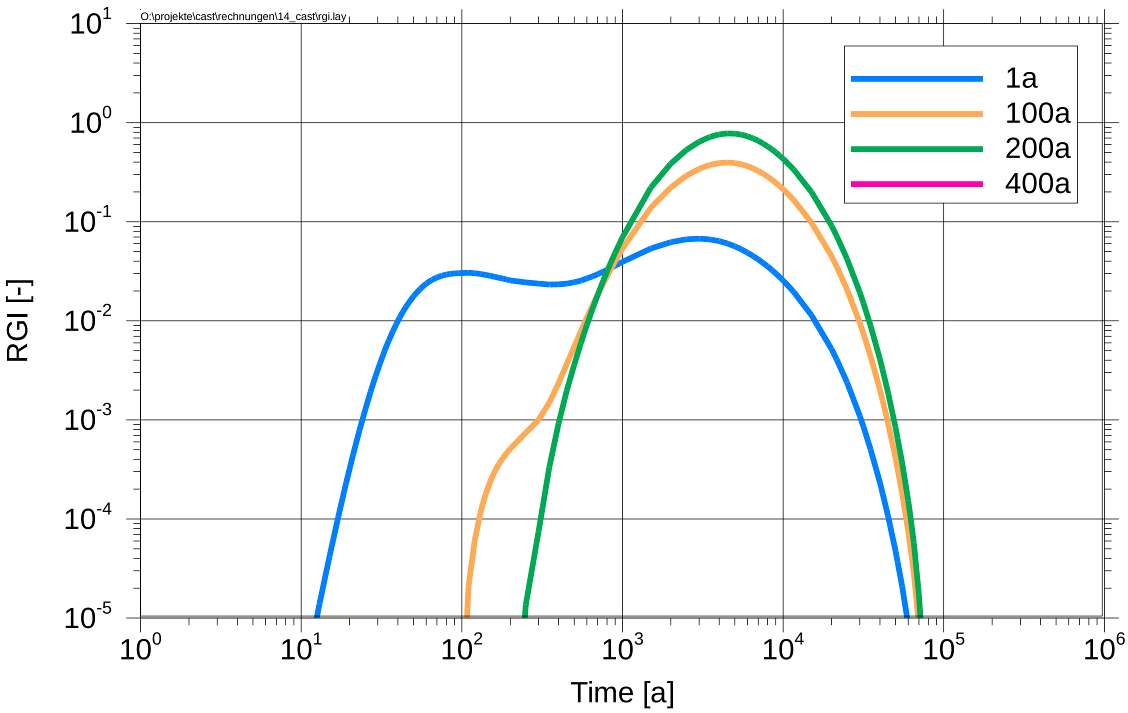


Fig. 2.21 Dependence of the radiotoxicity indicator RGI from the release start time

Fig. 2.19 shows the result of simulations varying the instant release fraction (IRF) of the ^{14}C. In the reference case of the VSG, a value of 20 % was used for metal parts and 10 % for Zircaloy and the fuel matrix. For the parameter variations performed in this project, values for the IRF of 10, 1 and 0.1 % were used equally for all types of wastes. The simulation results plotted in Fig. 2.19 show that a reduction of the IRF causes a reduction of the RGI by the same factor, suggesting a linear relationship of the IRF and RGI.

The first experimental results from CAST suggest values for the IRF in the range of 1 %, i. e. at the lower boundary of the range used in the parameter variations and therefore also much lower than assumed in the VSG reference case. However, the samples used and the type of experiments performed in CAST were not suitable to rule out the existence of a fraction of ^{14}C being initially in the gas phase of the spent fuel waste as a result of diffusion at high temperature from the waste as suggested by experiments reported in /SMI 93/. On the other hand, such type of gas phase was not found in experiments performed as part of the EC First Nuclides project which are reported by /KIE 14/. A maximum amount of only 0.2 % of the assumed ^{14}C inventory was found to be present initially in the gas phase of a fuel element tested in the First Nuclides project. As a result of both projects, First Nuclides and CAST it can be expected that the release of C-14 into the gas phase during the first 500 years under the assumed boundary conditions is lower than 10 % of the value assumed in the preliminary safety case for Gorleben or even less than 1 %. The reduction of conservatism in the assumption of the release behaviour of the IRF of ^{14}C in the waste is therefore a promising way to reduce the calculated RGI values in long-term safety assessment.

Fig. 2.20 shows the result of simulations varying the release rate of ^{14}C from the waste using values of 1, 10, 100 and 1 000 years for the time span of release. The release rate was considered to be constant in time throughout the respective periods. The curves plotted in Fig. 2.20 show that the RGI value is reduced somewhat at early times due to a slower release, however for late times the RGI value remains unchanged or is only slightly lowered. This is especially true for expected release times of some tens to a few hundred years at maximum.

Fig. 2.21 shows the result of simulations varying the start time of the ^{14}C release from the waste container using values of 1, 100, 200 and 400 years. As expected, a later start of the ^{14}C release also results in a later rise of the RGI value. For a start time of 400 years and later, no release of ^{14}C from the repository is occurring and the RGI value is consequently zero. The reason for this effect is that the convergence is already very low at that point in time and finally stops after 500 years. A subsequent gas transport therefore only occurs from pressure gradients already existing before that time. These pressure gradients are obviously too low to lead to a relevant gas transport after the convergence has stopped. More generally it can be pointed out that a ^{14}C release at a point in time where the porosity of the salt is close or even at its final value does not lead to a notable release from the repository. This clearly shows that the assumption of initially defect containers is critical for the ^{14}C release. A guaranteed container life-time of more than 500 years might prevent the release of gaseous ^{14}C from the repository.

As a summarizing conclusion it can be stated that the consequences of the ^{14}C release from the waste in the early phase of the repository, determined by the RGI indicator, are to a large part controlled by the quantity of the ^{14}C released. The temporal behaviour of the ^{14}C release only shows a minor impact on the RGI indicator. The potential to reduce the conservatism in the assumption of the amount of ^{14}C during the early phase of the repository is high according to the results obtained in the First Nuclides and the CAST projects.

2.4 Relevance of gases in the safety case

This chapter depicts a position paper developed by the Integration Group for the Safety Case (IGSC) /CAP 15/ summarizing and evaluating the current view on the role of gases in a safety case. The content is based on the summary of the general rapporteurs of the symposium of the European project “Fate of Repository Gases” (FORGE) /NOS 14/, which aimed to present salient results and key issues raised at the symposium and to place them in the perspective of the safety case. Account was further taken of key aspects discussed in a topical session (Thirteenth Meeting of the Integration Group for the Safety Case (IGSC), Topical session on the relevance of gas for the post-closure safety case of DGR for HLW and spent fuel, Paris, 19 October 2011) by the member organisations of IGSC.

2.4.1 Introduction

In the post-closure phase of a deep geological repository for radioactive waste, significant quantities of gases may be generated from various sources. The most important gas generating process is anaerobic metal corrosion. Additionally, degradation of organic matter by bacterial activity [mainly important for intermediate level waste and low-level waste (ILW and LLW) repositories] and water radiolysis contribute to gas formation. Non-radioactive gases can be important because of potential pressure related impacts on the engineered barrier system and geological host formation, and their role as a carrier gas for transporting radioactive gases. Repository designer may thus face a possible conflict of goals: while the design strategy of a disposal system is to provide isolation and containment, the non-radioactive gases may need to be dissipated to minimize any adverse effects from pressure build-up in the repository system.

Besides the large amount of non-radioactive gases, small amounts of radioactive gases are also generated and can have direct radiological consequences. Due to a usually large initial inventory and a longer half-life, ^{14}C if present in (or converted to) gas form can be of safety relevance depending on its degree and rate of conversion to methane and the period of confinement in the geological repository before it reaches the biosphere. Depending on the waste type, the concept and scenario, in some studies a fraction of volatile ^{129}I might be considered to be released from the waste. Radon presents a specific case as it will be continuously formed by radioactive decay of its parent nuclides during the containment period but also afterwards, when parent nuclides migrate throughout the barrier system. When applicable, ^{222}Rn is also particularly studied in the framework of operational period. Noble gases and tritium are not an issue for the post-closure safety due their short half-lives but may be considered for the operational period.

Gas production might also influence geochemical conditions in the near field and/or the host formation in different ways. A potential positive effect is a lower dissolution rate of spent fuel due to the reducing conditions imposed by the generation of hydrogen gas, while a potential negative effect could be a higher solubility of actinides due to the lower pH conditions imposed by the presence of gaseous CO_2. Consequently, a sound safety strategy addressing these issues and a body of robust arguments are needed to support a post-closure safety case in order to give an adequate level of confidence that gas generation is not an issue likely to compromise the safety of a deep geological disposal system.

Gas generation and transport in deep geological repository have been studied for more than 15 years in a series of successive international projects. These include the PEGASUS /HEI 96/, EVEGAS /MAN 97/, PROGRESS /ROD 00/ and the GASNET /ROD 03/ projects. A comprehensive review of several studies was also issued on this subject /ROD 99/. While R&D on gas issues continued from the early 2000s within the national programmes, there was a hiatus of several years for comprehensive multinational projects. In 2009, the FORGE (Fate Of Repository Gases) project, under the auspices of the European Commission, was launched with participants from radioactive waste management organisations, regulators and academia. In this context, the IGSC revisited the topic from a strategic point of view and issued this position paper to support the IGSC viewpoint, based on the results of the FORGE project /SHA 13/ and safety cases developed in various national programmes.

2.4.2 Gas sources in a deep geological repository

Gas generating processes in a repository include anaerobic metal corrosion, (bio-) chemical degradation of organics, and radiolysis of water and waste, from which gaseous radionuclides may also be released.

Corrosion processes of metal in geological repositories have been extensively investigated in many national programmes, with the objective to demonstrate that the containment requirement of radionuclides within the multiple engineered barriers can be met. R&D performed in the pursuit of that objective has also benefited to the evolution of the corrosion gas source term as advances in mechanistic understanding of the underlying processes have been achieved. Long-term corrosion experiments of steel exposed in conditions simulating a disposal system show carbon steel corrosion rates ranging from a few to tens of nanometres per year in cement-based systems, to tens of microns per year in bentonite-based systems /NAG 08/; /SER 10/; /NEW 13/. An asymptotic decrease of carbon steel corrosion rates has been observed in experiments and can be explained by the progressive passivation of steel where a protective corrosion product layer is formed on the canister surface. In the case of a copper canister, container lifetimes are very long, and gas generation rates are extremely low due to the thermodynamic stability of copper /KIN 10/.

Once confidence is established that metallic barriers can provide containment as required by the national regulations under stable conditions, R&D programmes tend to shift towards the study of corrosion processes under environmental conditions that will prevail during transients which immediately follow closure of the repository such as the re-saturation and/or the thermal phase. For heat-emitting wastes such as spent fuel, the thermal transient can extend over several centuries. Unsaturated conditions might also prevail for a significant period of time, depending on the type of host rock and the repository design. In some clay-based concepts, parts of the near field may remain only partially saturated for decades. Steel corrosion in an unsaturated, high humidity environment is not fully understood and few corrosion data are available. However, recent results for steel corrosion in cementitious material at 100 % humidity show corrosion rates similar to those observed in liquid water /NEW 13/. The effect of perturbations of the system after closure, such as the ingress of aggressive species, has also been investigated in several programmes /KUR 04/.

In some cases, availability of water might be a limiting factor for gas generation. This might apply in particular to repositories in dry host formations, like rock salt, for which unsaturated conditions are also expected to prevail for a significant time period after final closure /BEU 12/.

A variety of gases can be produced from radiolysis, hydrolysis and microbial degradation of cellulose, resins, bitumen and plastics present in low-level and intermediate-level, long-lived wastes (LLW and ILLW) /ROD 03/. Rates of gas generation from LLW under repository conditions have been quantified in large scale /ROD 00/; Molnar et al. /SHA 13/. A biogeochemical reaction-transport model of one such experiment has shown an estimate of gas production rate reasonably consistent with the test data

/SMA 08/. Nevertheless, the diversity of LLW and ILLW, the waste package heterogeneities, the evolving conditions of deep geological repositories and their possible local variability and microbial diversity in the environment are factors that would limit accurate predictions of the long-term gas generation rates in a repository.

Laboratory experiments have shown the remarkable adaptation behaviour and versatility of microbes in environments anticipated in a geological repository. Their possible impacts range from concrete carbonation through the production of CO_2 to the formation of volatile radioactive compounds via the methylation of iodine and selenium (Francis in /SHA 13/). Beyond the waste package, an adequately backfilled and sealed geological repository normally constitutes a harsh environment for microbes to be active, due to the lack of free space, slow diffusive transport of metabolites and often a lack of suitable carbon sources, electron donors or acceptors. Such environments are expected to severely limit, if not rule out, microbial activity, although supporting data are limited. It has been noted, however, that microbial activity can in some case be beneficial, e. g. certain microbes are capable of using hydrogen as a source of energy and therewith acting as a sink for hydrogen. Projecting longer term microbe behaviour for a specific repository setting encounters issues of variability and the long-term viability of microbes as the near-field environment stabilises.

2.4.3 Gas transport in deep geological repositories

Gas transport mechanisms are highly dependent on the type of host rock and the design and materials of the EBS (e. g. the type of backfill and sealing materials used).

In a disposal system saturated with groundwater (or close to saturation), dissolved gas can be transported via diffusion in pore water. No particular issues are expected for systems in which the gas generation rate is low enough for all gas to be continuously evacuated through this well-characterised process. Complexity – and differences between disposal systems – arise if the capacity for diffusive removal of dissolved gas is exceeded and a discrete gas phase is formed: characterisation of advective gas flow through natural or engineered low-permeability porous materials is a challenging endeavour, especially when those materials are close to saturation with water. For more than two decades, efforts to characterise gas transport modes have been pursued in laboratory and in situ tests while process models have been developed in parallel.

In the laboratory, the identification and characterisation of advective gas transport modes in small samples of natural or engineered low-permeability material is complicated by a high sensitivity of the results to the experimental conditions and the initial state of the samples /ROD 99/; /ROD 03/; /SHA 13/. Some of these conditions can be constrained by adequate control of the initial saturation, the stress or strain boundary conditions and the geometry of the experimental setup. Nevertheless, for natural materials, sample variability and interfaces with the experimental setup may still lead to very different results for otherwise similar tests: gas always takes advantage of heterogeneities to flow through the path of least resistance. For cementitious materials, large variability in gas migration properties might also show up as a result of sensitivities to manufacturing factors such as curing conditions and formulations /ROD 99/. An additional complexity presented by cement-based systems is the dynamic physicochemical evolution of the materials. This evolution can have different effects on porosity and gas permeability as these can be affected, for instance, by crack formation but also pore clogging due to formation of new phases.

In situ characterisation of gas transport in the host rock around underground laboratories presents additional challenges such as the presence of a disturbed zone around the experimental setup. Modelling studies reveal that the outcomes of such experiments are strongly dependent on the extent and the properties of this disturbed zone (Levasseur et al., Gerard et al., Granet and de La Vaissiére in /SHA 13/). A correct interpretation of in situ test results would thus ideally require an adequate characterisation of this zone. In absence of this, gas behaviour might be deduced from the injected gas volumes and observed pressures albeit with a considerable amount of uncertainties. After-test forensic analyses may also support the parameter identification process provided that the perturbations induced by gas transport can be distinguished from these resulting from the installation of the experimental setup.

2.4.3.1 Gas transport in clay systems

A large amount of laboratory experiments has been performed at the end of the last century to characterise the transport of gas under defined pressures through bentonite and other clay barriers (among others by /HOR 96/; /HOR 99/; /HAR 99/). These have been complemented by in-situ experiments and additional laboratory tests such as those reported in /ROD 03/. At the time, a consensus emerged among experimentalists that due to high gas entry pressures, the transport of gas through compacted clays saturated with water or close to saturation is only possible by the creation of specific gas pathways, i. e. a network of fissures or fractures. As a consequence, dilatant behaviour and the creation or reactivation of discontinuities in the material should be expected.

During the more recent FORGE project, additional laboratory and in-situ experiments on gas transport in clay systems (e. g. Birgersson and Karnland, Cuss et al., Harrington et al., Zhang et al., Graham et al., in /SHA 13/) have confirmed these earlier conclusions – dilation has been clearly evidenced in laboratory experiments on clays. Interestingly, the evaluation of water mass balances indicates no significant loss of water even after many hundreds of days of gas testing at elevated pressures, which strongly hints at separate gas- and water-filled networks.

Experimental evidence from in situ testing and laboratory tests performed on artificially damaged samples (Zhang et al., Svoboda and Smutek in /SHA 13/) confirm that around a repository, discontinuities in the disturbed zone can act as preferential gas transport pathways when a threshold gas pressure is reached, and these pathways may shut down once the pressure drops. Besides the disturbed zone, the possibility of localised gas transport along interfaces between repository components has also been identified (Popp et al. in /SHA 13/).

In laboratory tests, hydraulic conductivity measurements performed before and after gas flow generally do not exhibit notable differences. In situ, ample evidence has been collected of spontaneous sealing of discontinuities in confined, water saturated clay systems /SEL 07/; /TSA 11/; /LI 13/. A priori, discontinuities activated by gas transport should thus not act afterwards as preferential groundwater and solute transport pathways. This has been confirmed to be the case in the short term by in-situ experiments such as RESEAL /RES 09/. Given that gas release may spread over quite long periods, it should be checked, however, that other perturbations (e. g. alkaline plume) will not in the meantime negatively affect this “self-sealing” capacity.

Two-phase flow is a possible transport mode in materials with a lower gas entry pressure, such as sand-bentonite mixtures and possibly in some natural clayey formations at a large scale due to heterogeneities such as sandy facies. In these cases, it can be possible for a pressurised gas phase to displace porewater, without the creation of new, gas-specific pathways. Note that non-disruptive gas flow is also possible for materials with high gas entry pressures provided that the degree of saturation with water is low enough for continuous, water-free pathways to be maintained.

2.4.3.2 Gas transport in crystalline rock systems

For granite formations, the major concern with respect to gases is related to the integrity of the bentonite buffer, commonly used to protect waste containers in such formations. The gas transport processes in the buffer are those mentioned for a repository in clay but relevant parameter values like gas entry threshold might be different due to differences in structure and mineralogical composition. In a highly compacted bentonite buffer the gas entry pressure is high enough to prevent initiation of two-phase flow and dilation pathways are the main gas transport mechanism. In contrast to relatively tight clay formations, build-up of high gas pressures in granite formations is unlikely, since existing fractures already provide migration pathways for generated gases /SKB 11/. Therefore, a harmful effect of gases on the integrity of the granite host rock is not an issue. Further, the concepts followed in Sweden and Finland are based on copper canisters, where gas generation rates by corrosion are extremely low and without any negative consequences for the buffer. The iron insert of the copper canister may generate high amounts of gas by corrosion if the copper shell is damaged. Due to the high stability of copper it is expected that most of the canisters will stay intact within their typical design lifetime of 1 million years. The canister fabrication and sealing processes are expected to produce canister that are tight at deposition /SKB 11/. Defective canisters are not assumed to occur before 100 000 years after repository closure. In a scenario where a canister is damaged e. g. by an earthquake, but the buffer is intact, the buffer is expected to retain its properties throughout the gas-transport period so that gas-induced pathways are likely to close and seal when gas production ceases. Also, for hypothetical scenarios with an assumed number of canisters with a pinhole defect, the impact of gas formation is expected to be limited and local /SKB 11/. A pinhole is still a barrier in terms of allowing the movement of reactants and corrosion products, but typically very conservative assumptions are made in evaluating hypothetical initial defect scenarios.

2.4.3.3 Gas transport in salt systems

Due to the unsaturated conditions prevailing over very long times in the expected evolution of dedicated salt repositories, the process of gas dissolution does not play a major role. Gas transport is therefore dominated by advection in the gas phase. In case of low liquid saturation, gas can flow without needing to displace the liquid phase.

Rock convergence and subsequent compaction of crushed salt backfill are important processes in salt concepts. If backfill porosity is reduced to a few percent, saturation increases, and the vapour-liquid equilibrium may be shifted towards further gas dissolution. Rock convergence, gas and liquid flow are coupled processes: On the one hand convergence will increase the pore pressure and therewith initiate gas flow. On the other hand, the flow of gas will modify the pore pressure, and thus act on the compaction rate. This interplay can lead to a complex flow pattern inside a repository built in rock salt. Since convergence and compaction of crushed salt strongly depends on temperature, there is an initial gas flow from faster converging hot to slower converging cold areas. This implies that gas is accumulated in cold areas in which elevated pressures will evolve as soon as convergence progresses here, too. These effects have been observed in modelling studies for a hypothetical repository at the German Gorleben site /LAR 13/. Further, gas pressures might also act as a dynamic barrier by preventing liquids from entering the repository. However, many properties of highly compacted crushed salt backfill which are needed to quantify gas transport are still not well known.

The salt host rock itself is impermeable for gas at pressures well below the minimum principal stress.

Gas flow will therefore follow preferential flow paths given by the engineered barrier system (EBS), the excavation disturbed zones (EDZ), and material interfaces. Gas will cause macroscopic fractures in the host rock if gas pressure reaches the minimum principal stress of the rock. Due to stress heterogeneities at the microscopic scale gas will already infiltrate at slightly lower pressures on grain boundaries without compromising the host rock's integrity. It is important to mention that site-specific aspects may also play a crucial role. Indeed, a more heterogeneous formation such as the bedded Salado formation at the Waste Isolation Pilot Plant repository in New Mexico, USA, would allow gas to escape away from the repository along nearly horizontal higher permeability, but typically saturated, interlayers /NEM 10/.

2.4.4 Process level modelling of gas transport

2.4.4.1 Clay- and crystalline rock systems

Similar approaches are used for process-level modelling of gas transport through low permeability porous media such as EBS materials (bentonite in a crystalline rock) or the host rock itself (for a repository in clay). Conventional two-phase flow models are generally used to represent non-disruptive gas transport in porous media when the gas entry pressure is much lower than confinement stresses. If the gas pressure exceeds the minimum confinement stress, transport of gas occurs via the propagation of tensile fractures. The modelling of this transport mode is complex because initiation and propagation of discontinuities are intrinsically linked to the small scale local stress distributions, affected by the presence of heterogeneities. Several conceptual approaches have been proposed to represent disruptive gas transport /ROD 99/; /SHA 13/, one of these being two-phase flow models extended with semi-empirical hydromechanical couplings i. e. stress and/or damage-dependent transport properties.

Although these models may reproduce experimental observations to some extent, they rely on case by case tuning of the coupling parameters. To date, the large degree of freedom left to the modeller in the choice of parameters that cannot be directly measured (or which could only be obtained by destructive techniques) limits the predictive capability of such models. Models able to capture discontinuity creation and propagation caused by disruptive gas transport might remain out of reach because of the inherent limitations associated with the characterisation of natural porous media.

2.4.4.2 Salt systems

For salt repository concepts, the expected evolution is marked by very dry conditions. However, for less likely evolutions the possibility of brine intrusion has to be considered. Modelling fluid transport on the repository scale is a demanding task especially because of the interactions between flow and rock convergence mentioned before. In the nineties of the last century, these processes have been simulated by models that use networks of one- or zero-dimensional structures with sophisticated physical behaviour /HIR 99/; /MAR 02/. Such models are able to capture repository scale interactions with an affordable amount of calculation time but they usually do not fully incorporate the classical two-phase flow theory. Other approaches use standard two-phase flow codes that have been extended by processes that are typical to salt repositories /LAR 13/. Such models require a significant amount of calculation time and can be regarded as complementary to the before mentioned more efficient simplified model types.

Gas pressure as well as gas transport velocity strongly depend on porosity and liquid saturation. Even if the water content of crushed salt is very low, saturation will become relevant if the backfill porosity reaches the range between 0 % and 2 % in the long term. Also, pore structure and water mobility are not well known for low porosities so that the applicability of two-phase flow models for low backfill porosity conditions is still an open question. These aspects show that there is a general quantification problem in modelling gas transport in crushed salt used as a long-term sealing material in a converging host rock. This uncertainty has to be addressed in the safety assessment or the repository concept has to be changed.

The pore space of the backfill is not the only flow path for gas. Gas may also flow through excavation disturbed zones, along material interfaces and in some cases along the grain boundaries of undisturbed rock salt. All these pathways require different treatment according to their characteristic properties. Some aspects may be sufficiently covered by the classical two-phase flow theory. Others clearly call for enhanced modelling approaches. Classical two-phase flow models are less well suited if gas flow follows localised channels. Localised flow will occur along fractures and fissures of the excavation disturbed zone or along the interfaces connecting the seals with the host rock. Gas flows also tend to localise if preferential flow paths are opened by high pressures (“pathway dilation”).

The permeability of sealing materials like salt concrete or of discontinuities may depend on fluid pressure and the local stress state. In this case, hydro-mechanical models or two-phase flow models introducing a pressure dependency of permeability or permeability change are more appropriate.

2.4.5 Radiological impact

Gas can potentially affect the radiological consequences resulting from a deep geological repository in two ways. The first one corresponds to the direct release of radioactive gas itself. The second is of an indirect nature: if large amounts of inactive gas are produced in the repository, these might enhance radionuclide transport of dissolved radionuclides within the disposal system by displacing contaminated water, acting as carrier gas for volatile nuclides or inducing damage to the multi-barrier system as a result of excessive pressures.

Due to a potential large initial inventory and a longer half-life, gaseous ^{14}C can be of safety relevance depending on the period of confinement and transport of this gas in the geological system before it reaches the biosphere. The behaviour (e. g. solubility, transport) and impact (e. g. accumulation in the biosphere) of gaseous ^{14}C strongly depends on its speciation. The behaviour of ^{14}C is a matter of further research and will be addressed in the CAST project as part of the EC Seventh Framework Programme. Depending on the waste and the design, scenarios in which a fraction of volatile iodine can be released from the waste might also be considered. However, the contribution of radioactive gas to the total dose rate in the biosphere after closure is usually considered minor, except for dry systems in which radioactive gas releases can make up most of the radiological impact, e. g. /LAR 13/.

The influence of non-radioactive gas on radionuclide transport mainly depends on the balance between non-radioactive gas production rate and gas transport. If the gas production rate is low enough for the gas to be dissipated by dissolution in groundwater and diffusion, then the radionuclide transport in the liquid phase is not affected. If conditions in the repository are such that two-phase flow can develop, gas might displace contaminated pore water. In case of gas transport by pathway dilatancy, experimental evidence suggests that only little water is moving with gas in clay materials (Jacops et al. in /SHA 13/). Nevertheless, radioactive gas mixed with inactive gas will be transported during breakthrough events. After gas breakthrough, the well-documented self-sealing properties of a bentonite-based barrier and/or clay host rock should prevent the persistence of preferential pathways.

2.4.6 Treatment in safety assessment & management of uncertainties

The dominant gas generation process for geological disposal of vitrified high-level waste and spent fuel is anaerobic corrosion of steel. In performance assessment, the rate of gas generation by metal corrosion is generally determined as the product of the surface area and the corrosion rate. A large body of knowledge about metal corrosion rates in saturated systems is available /SMA 99/; /KIN 08/; /SHA 13/. Residual uncertainties on the actual conditions prevailing in the repository and their evolution in the long term shall be addressed in the safety assessment. Depending on the design, on the nature of the metal, and the host-rock the long-term corrosion rate of the metallic containers of HLW in saturated and non-disturbed disposal systems might be low enough so that all the generated gas can be fully evacuated by dissolution and diffusion alone. For LLW and some ILW, the accessible surface area of the metal is often conservatively estimated since they cannot be accurately determined, especially for older pre-packaged wastes. Gas-generation and transport modelling results based on such estimates will likely overstate the potential importance of the gas generation and transport processes.

Gas generation in unsaturated systems, such as in salt formations, may be limited by the availability of water.

Diffusive transport of dissolved gas through groundwater is a well understood and easily modelled mechanism. Models are also available to represent two-phase flow when it applies. For low permeability clayey material and for very low porosity and low permeability materials like compacted salt grit, there are conceptual limitations to developing a hydro-mechanical model able to capture gas flow through dilatant pathways. Extension of two-phase flow models coupled to mechanical poro-elasto-plastic/damage models calibrated with available in situ measurements might circumvent these limitations to some extent and provide a tool for use in a safety assessment provided that simplifying assumptions and their conservatism are documented and remembered in interpreting results.

In addition to the epistemic uncertainties that may be reduced by more characterisation efforts, gas transport through discrete features suffers also ontic – irreducible – uncertainties due to the complexity of some of the processes and features involved, such as damage propagation and pathways instability. In order to account for this inherent limitation, different strategies exist. With respect to the source term, uncertainties can be reduced by the estimation of more realistic corrosion rates, dissolution rates, and specific surfaces. A second option is to optimise the design of the repository, by (i) minimising the amount of gas producing materials, and/or (ii) minimising gas generation rates by optimisation of geochemical conditions and/or (iii) limiting the availability of water within the engineered barrier system.

Comparable strategies can be followed with respect to gas transport. A reduction of the uncertainty associated with complex gas transport modes might be sought through the choice of EBS materials through which gas transport can be more easily characterised. The design for gas transport might be optimised by maximising the exchange surface for transport of dissolved gas, i. e. adapting the repository geometry and/or organising storage & transport capacities to cope with gas production rates, e. g. by the choice of porous, non-compacting backfilling material, or by explicitly providing long-term stable gas evacuation pathways, e. g. Engineered Gas Transport System (EGTS) /NAG 08b/.

2.4.7 Importance for the safety case

Repositories are designed to contain radioactive materials for as long as is possible. Gas generation and the physical processes it may induce ought not determine repository safety but may be a contributing factor. Even if it is not a primary determinant of safety, it may still be a source of an unwelcome degree of uncertainty.

The foregoing discussion has described, based on decades of previous work, the state of the art in considering gas generation, evolution and transport in the context of deep geological repository system performance. Uncertainties in modelling gas-related processes have been discussed, as have strategies for dealing with uncertainties through doing more scientific work, redesigning the repository, or operationally controlling the content of the repository.

Determining whether or not such additional scientific, design or operational control activities need to be undertaken is aided by sensitivity analyses. If overall repository safety is not strongly dependent on processes related to gas generation and transport, then existing information may allow a case for repository safety to be credibly made based on conservative modelling of gas generation and transport processes. Long-term gas-process related effects on repository performance must be evaluated in the context of applicable safety requirements. In instances where requirements are likely to be met, a conservative gas generation and transport approach in the context of a comprehensive safety case can convince the implementer, key stakeholders and regulators to allow the project to move forward in its evolution.

If gas-generation and transport processes are relatively important to determining long-term repository safety, then there are options to be considered to reduce uncertainty and thereby allow more realistic safety evaluations to be done or redesigning the proposed repository system. Beyond the implementer’s conviction, the confidence in uncertainties management in the safety case should be shared by regulator and other stakeholders. A strategy for obtaining a broader base of support for a construction license may include scientific or design work to reduce uncertainties in order to meet their expectation.

2.5 Treatment of uncertainty

The assessment of the post-closure radiological consequences forms the core of the safety case for a radioactive waste disposal facility. This involves a comprehensive approach for the handling of the uncertainties. Besides the uncertainties about the future evolution of the repository system as described in Chapter 2, uncertainties about the model parameters used in long-term safety assessment are of high relevance. Such uncertainties can be addressed directly in the calculations via deterministic and/or probabilistic approaches.

This topic is continuously further developed and an issue of international cooperation. With this respect a series of workshops have been performed during the last years in order to compile the current status of strategies and methods used and identify topics for further cooperation. A description of the outcome of a workshop in UK is given in Chapter 2.5.1 and the status of an international collaboration which was started in 2017 is given in Chapter 2.5.2.

2.5.1 International workshop and cooperation

A two-day workshop was held at RWM offices in Harwell, Oxford, as an initiative to enable technical information exchange between radioactive waste management organisations on topics around the treatment of uncertainty in post-closure safety cases. There were 16 participants, representing nine different international programmes. The workshop provided a forum to understand how the work developed during earlier projects, for example the EC PAMINA project and NEA MeSA project, is now being applied to safety cases in national waste management programmes. A key aim was to identify areas, where further developments may benefit the safety case in order to explore the potential for collaboration in this area.

Three main topics were discussed:

- quantification of uncertainty,
- modelling issues, and
- sensitivity analysis.

The first session dealt with quantification of data uncertainty and expert elicitation. It was explained that most people (including scientific experts) display bias when eliciting uncertainties, typically reflecting over-confidence. A number of elicitation methodologies have been developed to help avoid such biases. For example, bias can be reduced by providing training to experts using examples of uncertainty in everyday life and through the use of a structured methodology. RWM developed a simple tool (implemented in Microsoft Excel) designed to help experts to quantify uncertainty in a structured way and hence derive more appropriate PDFs for use in safety assessments. It was noted that expert quantification of uncertainty could be both expensive and resource-intensive. A multi-level approach was proposed in which the effort expended should be linked to the importance of a parameter, the quantity of available evidence and the stage of the programme. Important questions in this context are, e. g.:

- What are the pros and cons of each existing elicitation methodology?
- Are there examples from other fields where elicitation has successfully been applied previously?
- Would a structured method for uncertainty quantification be useful in the field of radioactive waste management?
- How should correlated uncertain data be treated?
- Could a toolkit be designed to build confidence with stakeholders? Popular science books, for example Daniel Kahneman's book 'Thinking, Fast and Slow', may also help with this.
- How do national regulations affect the treatment of uncertainty?
- Do different types of uncertainty need to be distinguished?
- When should logarithmic scales be used for PDFs?
- Does an expert elicitation require a different type of meeting from developing a conceptual model?

There was a general consensus that the development of a well explained, effective and proportionate methodology for uncertainty quantification would be of benefit to safety assessments. This should take note of the fact that different programmes are at different stages of development and have different regulatory expectations and should therefore not be overly prescriptive.

With respect to modelling issues it can be concluded that some organisations actively applied and refined techniques and methods developed and tested throughout the PAMINA project. This was illustrated by presentations from NAGRA, GRS and SANDIA presenting the application of screening methods (e. g. Morris one-at-a-time), Monte-Carlo based methods (e. g. rank correlation coefficients) and variance-based methods (e. g. Sobol indices), the development of new statistical tools, and application of 3D Multiphysics models, respectively. Discussion after the presentations considered the following questions:

- Are techniques for uncertainty propagation and sampling (e. g. convergence tests, use of Latin Hypercube Sampling) now standardised?
- How can conceptual model uncertainty be treated appropriately?
- Is it still useful to make a distinction between detailed 'process level' models and abstracted 'system level' performance assessment models? Is there now a trend for the two to merge, and if so is this a good or a bad thing?
- Is it actually beneficial for waste management organisations to develop their own individual codes, so that results can be independently benchmarked?

Views differed among the attendees about the merging of process and system level models, however there was agreement that the most important aspect of modelling is to build and demonstrate understanding. That understanding can be obscured by developing overly complex models and computing power is no substitute for proper scientific thinking. However, it was also noted that the production of abstracted system models may not be possible in all situations (especially where there are coupled non-linear physical processes at work) and that the extent to which this is the case depends on the nature of the studied system, i. e. of the repository concept among other things. In all cases, what really matters is to gain sufficient understanding to produce a robust safety case, recognising that the numerical modelling is just one component of the safety case. Given the nature of the codes required, there may be opportunities to share effort on the development of new multi-physics codes or to benchmark existing codes against one another.

In the session on sensitivity analysis presentations regarded recent academic trends in sensitivity analysis, such as visualisation techniques, including scatterplots and CUSUNORO curves, variance-based methods and methods using fuzzy set theory. Problems related to non-linear and non-monotonic behaviour of repository systems

(e. g. in rock salt), in which parameter sensitivities vary strongly with the values of other parameters and output values vary widely and can even include zero results, were also addressed. The discussion after the presentations addressed:

- How can correlated input data be treated in sensitivity analyses?
- What is the best way to present the results of sensitivity analyses?
- Could a standardised approach to sensitivity analysis be produced? Would such guidance help to convince a regulator that appropriate techniques had been used?

There was a general consensus that there is already a relatively well-stocked ‘toolbox’ of techniques for sensitivity analysis, although no single technique is suitable for all models and applications. With respect to this topic, co-operation between some of the participating organisations will be sensible. Such a co-operation could include analysis of existing WIPP data with the different sensitivity analysis methods presented as well as benchmarking the probabilistic tools on the basis of a WIPP-based system. Further work on treating correlated input data may also be beneficial to the safety case.

All attendees agreed that the workshop had been extremely beneficial. There was excellent information exchange and discussion, including the identification of specific further areas of possible collaboration and information exchange between certain participants. It was agreed that further collaboration on methods for quantifying uncertainties (for example further trial and development of the uncertainty quantifier spreadsheet tool) would be beneficial. The ultimate goal would be to work towards developing an effective, intuitive, proportionate and well-explained methodology for uncertainty quantification that is accepted internationally by relevant academics and regulators and, ideally, used both within and outside radioactive waste management.

2.5.2 Methodological investigation of uncertainty and sensitivity analysis for final repository systems in international comparison

In many countries, probabilistic uncertainty and sensitivity analysis is considered an essential tool for analysing numerical models for repository performance assessment. Specifically, sensitivity analysis can yield valuable information about the model behaviour and help improving system understanding. However, various different mathematical approaches are used for this purpose, producing results that are not always completely comparable or tell the same story about the system.

Within the project MOSEL /SPI 17/ different methods of probabilistic sensitivity analysis were applied to typical repository system models and analysed with respect to their usefulness in practice and their different messages. Four types of sensitivity analysis methods were investigated:

- graphical methods,
- non-parametric analytical tests,
- regression- or correlation-based methods, and
- variance-based methods.

It turned out that the different types of methods perform differently well on repository PA models. A model incorporating distinct nonlinearities and even discontinuities was most demanding and required many thousands of model runs to achieve stable and plausible results.

In many other countries probabilistic uncertainty and sensitivity analysis for repository models has been performed for decades. Specifically, in the USA, there is considerable experience with probabilistic investigations for the Yucca Mountain and WIPP sites. The applied approaches, however, differ from those considered in MOSEL.

In August 2017, a 3-day-workshop on uncertainty quantification was organised by Sandia in Albuquerque, New Mexico. Apart from US scientists, participants from GRS, TU Clausthal (both Germany) and RWM (UK) attended the workshop and discussed methodological and practical aspects of uncertainty quantification in the context of radioactive waste management. While the first day was dedicated to the expert elicitation techniques and tools developed by RWM – see previous chapter – and the third day dealt with uncertainty management for the WIPP site, the second day was focused on sensitivity analysis. Methods and tools for sensitivity analysis applied in Germany and the USA as well as application cases were presented and discussed. While in the USA there is large experience with detailed and elaborated sensitivity analyses for the WIPP site, mainly applying well-established methods, the research in Germany during the recent years was more focused on methodological aspects. It was found that an exchange of experience in form of a benchmark exercise would provide a good chance to learn from each other.

Therefore, a collaboration was agreed to compare the approaches and results. After the workshop, groups from Belgium and Finland joined this cooperation.

It was agreed, in order to keep the effort manageable, to start with existing probabilistic data from recent calculation cases of the participants. As a first step, a questionnaire was prepared for identifying such calculation cases. Six appropriate systems (3 from USA, 2 from Germany, 1 from Belgium) were identified.

The work reported in the following comprises two tasks, aiming at preparation of a detailed comparison of probabilistic approaches applied in different countries.

1. In MOSEL, no practically applicable method for computing variance-based sensitivity indices of the second order could be identified, and the available methods for total-order indices did not perform satisfyingly. As these indices are expected to provide valuable information about the behaviour of a model, this gap should be closed. Some promising first results were achieved with the RS-HDMR meta-modelling approach. It is planned to bring this into the international comparison exercise, but prior to that, some more detailed investigations with the models used in MOSEL were necessary to gain more understanding of the method and its application.

2. Between the participants of the planned exercise several comparison cases, based on the national programmes, were agreed for investigation. Some orienting computations were performed.

2.5.2.1 Second- and total-order sensitivity analysis using the RS-HDMR meta-modelling approach

Variance-based sensitivity analysis is based on the idea of decomposing the model output f into contributions depending on the input parameters x_i . This is called the ANOVA-HDMR decomposition:

$$f(x_1, x_2, \dots, x_n) = f_o + \sum_i f_i(x_i) + \sum_i \sum_{j>i} f_{ij}(x_i, x_j) + \cdots + f_{12\dots k}(x_1, \dots, x_n) \qquad (2.2)$$

It is known that this decomposition is unique if the mean value of each term with respect to integration from the set of any variable it depends on is equal to zero, in which case pairs of component terms are orthogonal with respect to integration /SOB 01/. Under the assumption that this is valid, the variances of the terms in the ANOVA decomposition add up to the total variance of the function

$$\sigma^2 = \sum_{s=1}^{n} \sum_{i_1 < \cdots < i_s} \sigma^2{}_{i_1 \dots i_s} \qquad (2.3)$$

where $\sigma^2{}_{i_1 \dots i_s} = \int f^2(x_{i_1} \dots x_{i_s})$ are known as partial variances. The global sensitivity indices are defined as the ratios $S_{i_1 \dots i_s} = \sigma^2{}_{i_1 \dots i_s} / \sigma^2$, from which follows that the sum of all sensitivity indices is always 1.

The indices $S_1 \dots S_n$ are called first-order sensitivity indices. They quantify the influences on the model output for which the respective parameters are alone responsible. Higher-order indices quantify the influences of parameter combinations. The sum of all indices containing contributions of parameter j is called the total-order sensitivity index of that parameter:

$$ST_j = \sum_{s=1}^{n} \sum_{\substack{i_1 < \cdots < i_s \\ j \in \{i_1 \dots i_s\}}} S_{i_1 \dots i_s} . \qquad (2.4)$$

It quantifies the total influence of parameter j on the model output in combination with all others. A clear difference between first- and total-order indices is always a sign for considerable parameter interactions.

In MOSEL, only first- and total-order sensitivity indices were considered. For calculating first-order indices a number of methods are available, which perform differently well. The EASI method (Effective Algorithm for calculating global Sensitivity Indices, /PLI 10/) is numerically effective, applicable with any kind of sampling, and produces consistent results with reasonable numbers of runs, even for a highly nonlinear model. It is, however, not able to calculate total-order indices. In principle, this is possible with the original Sobol' method /SOB 01/, /KUC 17/, but in MOSEL it was found that, at least with the mentioned nonlinear model, this technique does not produce convincing results with a manageable number of runs. The only practically applicable possibility to calculate total-order indices that could be identified in MOSEL was the EFAST method (Extended Fourier Amplitude Sensitivity Test). This method, however, requires a specific periodic sampling that provides a rather inhomogeneous coverage of the parameter space. Alongside other disadvantages like non-reusability of samples, this seems to be the reason for the observed low robustness of the method; the results turned out to be sensitive to the random seed of the sampling procedure. A robust method for computing total-order indices could not identified in MOSEL.

The RS-HDMR approach is based on meta-modelling and can compute sensitivity indices of first, second and total order on the basis of random or quasi-random sampling. Therefore, it is a candidate method for closing the mentioned gap. The investigations described in the following aimed at testing how this method performs with the nonlinear and discontinuous model used in MOSEL.

2.5.2.1.1 The RS-HDMR method[1]

The RS-HDMR method exploits the fact that for many practical problems only low order interactions of input variables have a significant impact on the model output /RAB 99/. It can dramatically reduce the computational time for building meta-models /LI 06/.

Assuming that component functions in (1) are piecewise smooth and continuous, they can be decomposed using a complete basis set of orthonormal polynomials:

$$f_i(x_i) = \sum_{r=1}^{\infty} \alpha_r^i \, \varphi_r(x_i) \, , \tag{2.5}$$

[1] The authors thank Sergei Kucherenko for providing this chapter.

$$f_{ij}(x_i, x_j) = \sum_{p=1}^{\infty} \sum_{q=1}^{\infty} \beta_{pq}^{ij} \, \varphi_{pq}(x_i, x_j) \,, \tag{2.6}$$

and so on. Here $\varphi_r(x_i), \varphi_{pq}(x_i, x_j)$ are sets of one- and two-dimensional basis functions and α_r^i and β_{pq}^{ij} are the coefficients of decomposition. From the orthogonality of the basis functions it follows that:

$$\alpha_r^i = \int_0^1 f_i(x_i) \, \varphi_r(x_i) dx_i, \qquad r = 1, \dots k, \tag{2.7}$$

$$\beta_{pq}^{ij} = \int_0^1 \int_0^1 f_i(x_i) \, \varphi_p(x_i) \varphi_q(x_j) dx_i dx_j, \quad p = 1 \dots l, q = 1 \dots l'. \tag{2.8}$$

The choice of the basis functions depends on the probability distributions of the inputs (i. e. for uniformly distributed inputs the suitable basis is Legendre polynomials). In the case of arbitrary distributions, a common practice is to use variables transformation to transform a given distribution to a uniform distribution (as described e. g. in /ZUN 13/).

For practical purposes the summation in (2.5) and (2.6) is limited to some maximum orders k, l, l':

$$f_i(x_i) \approx \sum_{r=1}^{k} \alpha_r^i \, \varphi_r(x_i) \tag{2.9}$$

$$f_{ij}(x_i, x_j) \approx \sum_{p=1}^{l} \sum_{q=1}^{l'} \beta_{pq}^{ij} \, \varphi_p(x_i) \varphi_q(x_j) \,. \tag{2.10}$$

Hence, the HDMR approximation function up to the second order interaction can be constructed as

$$\tilde{f}(x) = f_o + \sum_{r=1}^{k} \alpha_r^i \, \varphi_r(x_i) + \sum_{p=1}^{l} \sum_{q=1}^{l\prime} \beta_{pq}^{ij} \, \varphi_p(x_i) \varphi_q(x_j) \,. \tag{2.11}$$

The error of the model approximation is measured by the scaled L^2 distance:

$$\delta(f,\tilde{f}) = \frac{1}{\sigma}\int \left[f(x) - \tilde{f}(x)\right]^2 dx\,. \quad (2.12)$$

We note that $\delta(f,\tilde{f})$ has a link with the statistical fitness measure R^2 by the relationship $\delta(f,\tilde{f}) = 1 - R^2$.

An important problem is the choice of the optimal polynomial orders in equations (2.9) - (2.10). Ziehn and Tomlin /ZIE 08/, /ZIE 09/ proposed to use a least squares minimization technique in determining the optimal polynomial order for each component function. Zuniga et al. /ZUN 13/ proposed the use of the convergence of the sensitivity indices in defining optimal polynomial orders for each component function.

The coefficients of decomposition can be estimated by two different techniques. The first one, known as the projection method is a direct estimation of the integrals (2.7) - (2.8) by integration schemes (Monte Carlo / Quasi Monte Carlo, multivariate Gauss quadrature techniques, etc.). Li and Rabitz /Li 06/ proposed the use of ratio control variate methods to improve the accuracy of estimation of the coefficients of decomposition. Zuniga et al. /ZUN 13/ used QMC based on Sobol' (LpTau) sequences for improving the accuracy of integration. They also proposed determining an optimal number of points such that the variance in α_r^i as a function of N in two consecutive simulations was within some tolerance. The second method, generally known as the regression method, is based on estimating the PCE coefficients by minimizing the mean square error of the response approximation /ZIE 08/, /ZIE 09/. The higher the number of component functions in the truncated expansion, the higher will be the number of sampled points N needed to evaluate the polynomial coefficients with sufficient accuracy. Different methods have been proposed to build a sparse PCE in order to minimize N and the discrepancy between $f(x)$ and its polynomial chaos expansion approximation /SUD 00/, /SUD 08/.

Coefficients of the decomposition can be used to evaluate Sobol' sensitivity indices /LI 02/ as

$$S_i \approx \frac{\sum_{r=1}^{k}\left(\alpha_r^i\right)^2}{\sigma^2} \quad (2.13)$$

$$S_{ij} \approx \frac{\sum_{p=1}^{l} \sum_{q=1}^{l'} \left(\beta_{pq}^{ij}\right)^2}{\sigma^2} \tag{2.14}$$

This method of Sobol' sensitivity indices computation is used in the SobolGSA software.

2.5.2.1.2 Investigation of RS-HDMR with a nonlinear repository model

For the investigations described here a generic model for simulation of the contaminant release from a repository for Low- and Intermediate-Level Radioactive Waste (LILW) was used. It is assumed to be established in an abandoned former salt production mine. The model includes some relevant properties of a model for an existing site in Germany. As the mine was not specifically designed for waste disposal, specific measures need to be taken to stop or reduce undesirable processes. This includes the construction of a seal in the near field, which, however, is subject to chemical corrosion under the influence of brine and therefore only effective for some limited period of time. The model is rather complex and exhibits a highly nonlinear, non-monotonic and partly discontinuous behaviour. It is subject to many parameter uncertainties.

The model is described in detail in /SPI 15/; in the following, only a short overview of its features is given. Fig. 2.22 presents a schematic view of the model structure. The near field consists of four model compartments: two emplacement chambers (AEB and NAB), a mixing tank (MB) and a large area of mine openings with no waste (RG). One of the emplacement chambers (AEB), which contains the most long-lived radionuclides, is sealed from the rest of the mine. The mixing tank is connected to the far field model.

For simplicity, it is assumed that the non-sealed part of the mine is filled by brine instantaneously at some specific point in time. Beginning at this point in time, the brine percolates gradually into the sealed emplacement area AEB. In reality, there would be a slow brine intrusion to the mine building, triggering a slow increase of the fluid level and a time-dependent dissolution of the contaminants.

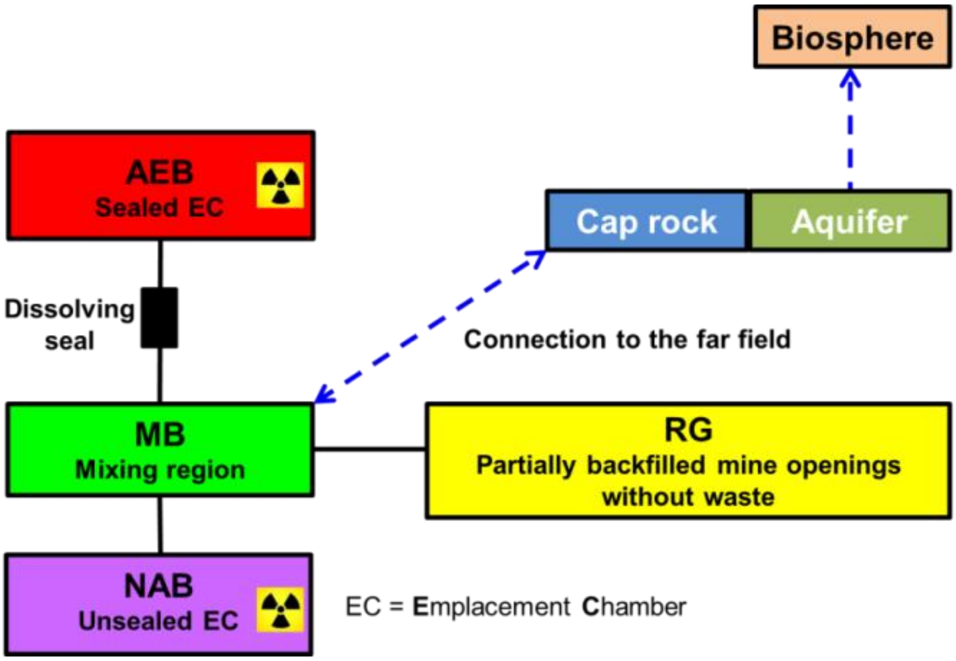


Fig. 2.22 Schematic view of the components of the LILW system

An important characteristic of the model is the seal between AEB and MB. It represents a sealing construction consisting of salt concrete, which is subject to chemical dissolution (corrosion) by magnesium-containing brine. It is assumed that the corrosion front proceeds gradually through the seal, which leads to loss of its isolation capability nearly suddenly at some point in time, resulting in a significant change of the model behaviour and usually a rise of the radiation exposure. A number of parameters determine the time of seal failure. With respect to some of these parameters, the model behaves nearly discontinuously when analysed at a specific point in time.

The seven most influential parameters are shown in Tab. 2.3; all others were fixed to their reference values. One parameter, *BrineMgSat*, has a distinctly right-skewed triangular distribution and its reference value is clearly different from its mean. This leads to different system behaviour and different sensitivities, depending on whether the parameter is varied or fixed. Therefore, two variants of the LILW model are considered, one with variation of six parameters and *BrineMgSat* fixed to its reference value 0.1 (LILW6) and one with variation of all seven parameters (LILW7). Physically, *BrineMgSat* defines the magnesium saturation in the corrosive brine in the repository mine in relation to that of IP21 solution.

Tab. 2.3 Parameters of different LILW models (LILW6 = red, LILW7 = red + green) and their distributions /SPI 17/

Parameter	Type of pdf	Range or pdf parameters	Reference value
GasEntryP: Gas entry pressure	Uniform	0 - 2.5	2.0
IniPermSeal: Initial permeability of dissolving seal	Log-normal	μ=41.0605 σ=1.9809	$1.0 \cdot 10^{-18}$
RefConv: Reference convergence rate	Log-uniform	$1.0 \cdot 10^{-5}$ - $1.0 \cdot 10^{-4}$	$4.0 \cdot 10^{-5}$
AEBConv: Factor of local convergence variation in AEB	Log-uniform	0.05 - 5.0	1.0
GasCorrPE: Organics corrosion rate	Log-normal	μ=12.6642 σ=1.1177	$1.0 \cdot 10^{-5}$
TBrine: Time of brine intrusion	Log-normal	μ=8.8857 σ=0.6933	7500
BrineMgSat: Relative magnesium saturation of brine	Triangular	0 - 0.1 - 1.0	0.1

As the model output the radiation exposure of a man was calculated with the RepoTREND package /REI 16/, /REI 17/, using the program modules LOPOS, GeoTREND-SP and BioTREND for the near field, the far field and the biosphere. For a time-dependent analysis, 31 time points, distributed over one million years, were used.

The RS-HDMR approach needs to be adjusted using the parameters k and $l = l'$, which denote the maximum considered orders of the coefficients alpha and beta (α_r^i and β_{pq}^{ij}), see equations (2.9) and (2.10). For the tests presented here the maximum polynomial orders $k = 10$ and $l = 4$ were used in (2.9), (2.10), which turned out to be reasonable in most cases.

For comparison, the results of two other methods for calculating sensitivity indices were used: the EASI method /PLI 10/ and the SDP approach /RAT 06/, /RAT 07/. The idea of EASI is to introduce periodicity into a parameter sample by re-ordering and perform a Fourier analysis on the model output. SDP is, like RS-HDMR, based on meta-modelling. Both methods are capable of calculating first-order sensitivity indices and have already been investigated in MOSEL. All considered methods, RS-HDMR, EASI and SDP, work, in principle, with any kind of sampling. Since quasi-random Sobol' LpTau sampling were found to yield the most robust results, it was used for the following tests. All investigations were carried out with subsets of an LpTau sequence of 16384 data points.

2.5.2.1.3 Results

Sensitivity index of the first order (SI1)

A very good agreement of the time-dependent SI1 curves was obtained for the LILW6 model from the RS-HDMR approach using SobolGSA compared to those attained from SDP and EASI (Fig. 2.23). For the LILW7 model, there are some small deviations for the parameter *IniPermSeal* starting at about 10^5 years. This leads to the hypothesis that these deviations are enhanced when the parameter *BrineMgSat* has a tendency to higher values. *BrineMgSat* does not show up as significant itself but causes great influence upon the two most important parameters (*IniPermSeal* and *AEBConv*). The probability of seal failure before a specific point in time increases if the parameter *BrineMgSat* has a higher value, which is the case in most runs of the LILW7 model compared to the LILW6 model. As a result, the second parameter impacting this probability, the initial seal permeability *IniPermSeal*, gets less significant for the LILW7 model. Once the seal has failed, the influence of the convergence rate of the sealed emplacement area, *AEBConv,* upon the release of contaminants increases while that of *IniPermSeal* decreases.

The instability of the SI1 of *TBrine* for both LILW models before 10^4 years is a result of the fact that this parameter, which defines the time of brine intrusion to the mine, controls the start of the model output, since contaminant release can and will only happen after the time *TBrine*. At early times there are only a few cases with nonzero model output values, providing a small statistical basis and a very small variance from which the sensitivity indices are computed. At very late times *TBrine* has very little influence, resulting in a small conditional variance. SDP has apparently difficulties in dealing with small values of the output.

For the LILW6 model, Fig. 2.24 shows how the calculated first-order indices converge with increasing number of model runs. With 512 runs, the time curves look uneven and agree only roughly between the three methods, but specifically for RS-HDMR they deviate significantly from those calculated with 8 192 runs (Fig. 2.23, left). Obviously, a few hundred runs are not sufficient for a proper first-order sensitivity analysis of this model. The curves calculated with 4096 runs, however, are in good agreement between each other and with those of Fig. 2.23.

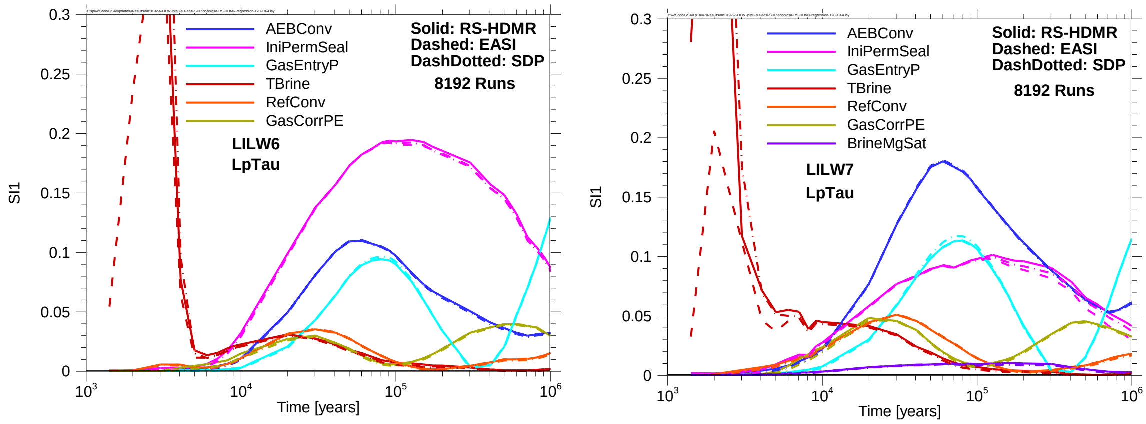


Fig. 2.23 Sensitivity index of the first order (SI1) of the LILW6 and LILW7 models obtained by the different approaches

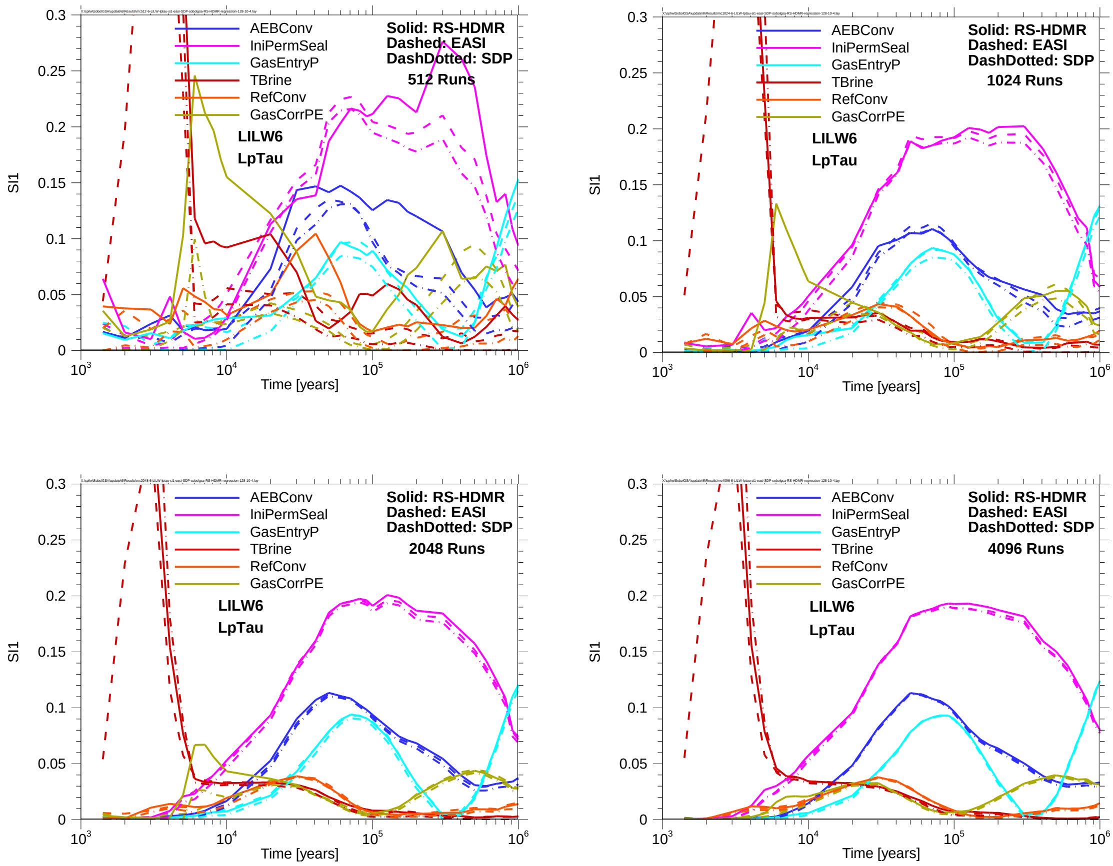


Fig. 2.24 Sensitivity index of the first order (SI1) of the LILW6 model obtained by the different approaches and different number of simulations (sets with 512, 1 024, 2 048 and 4 096 simulations)

It can be seen at Fig. 2.23 and Fig. 2.24 that the agreement between the three methods applied with the same sample size is generally better than that between evaluations using the same method but with different sample sizes. Since all evaluations with the same sample size were done utilising identical subsets of the total set of 8 192 runs, one can conclude that the concrete positions of the sample points in the space of parameter values is more relevant for the shape of the SI1-curves than the method of evaluation.

Sensitivity index of total order (SIT)

The time-dependent SIT curves indicate the importance of the different parameters in interactions with other parameters (Fig. 2.25). For the LILW7 model, the parameter showing the most important interactions with other parameters is *AEBConv*, followed by *GasEntryP, IniPermSeal*, *RefConv* and *GasCorrPE*. This can be seen by subtracting SI1 from the respective SIT of the same parameter. The high significance of *AEBConv* is understandable as there is an increased probability of seal failure compared to the LILW6 model because of higher values of *BrineMgSat*. Thus, *AEBConv* also controls interactions with other important parameters. The first order analysis already indicated that *AEBConv* was the most important parameter for the LILW7 model. *TBrine* plays a role in interaction with other parameters only at the beginning, which is plausible, as this parameter defines the start of contaminant release. *BrineMgSat* only shows little interaction effects with other parameters. For the LILW6 model, *AEBConv* also shows important interactions but lower than for the LILW7 model. *GasEntryP, RefConv* and *GasCorrPE* do not show many differences in importance between both models.

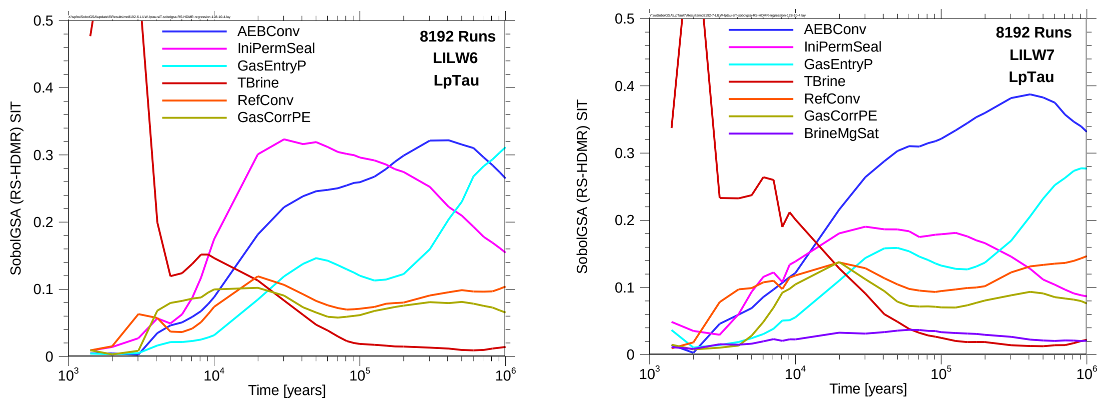


Fig. 2.25 Sensitivity index of total order (SIT) of the LILW6, and LILW7 models obtained by the RS-HDMR meta-modelling approach

Sensitivity index of second order (SI2)

The results of the second-order analysis obtained with RS-HDMR using the SobolGSA software indicate that different models include interactions between two parameters in particular with regards to the controlling parameter after seal failure, *AEBConv*, and the following most important parameters (Fig. 2.26): *GasEntryP*, *RefConv*, *IniPermSeal* and GasCorrPE, i. e., ([AEBConv] [*GasEntryP*]), ([*AEBConv*] [*RefConv*]), ([*AEBConv*] [*IniPermSeal*]) and ([*AEBConv*] [*GasCorrPE*]). The brackets around each of the two parameters indicate the presence of interaction effects between them. While for the LILW6 model the influence of the interaction ([*AEBConv*] [*IniPermSeal*]) is higher than for the LILW7 model, the opposite is valid for the interaction ([*AEBConv*] [*RefConv*]). The first order analysis also demonstrates that for the LILW6 model, compared to LILW7, the influence of IniPermSeal is higher and that of *RefConv* is lower. An important interaction at the beginning of the simulation is *TBrine* with *IniPermSeal*. These results are justifiable from the physics point of view.

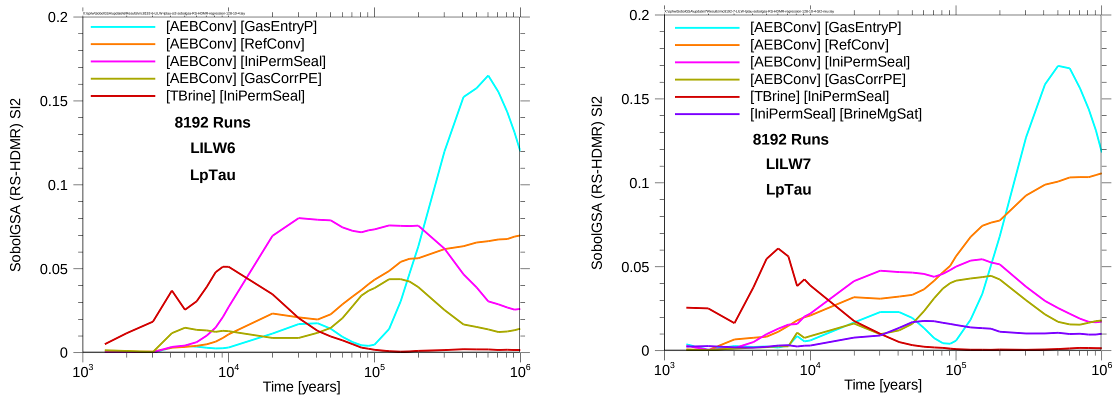


Fig. 2.26 Sensitivity index of second order (SI2) of the LILW6, and LILW7 models obtained by the RS-HDMR meta-modelling approach

Sum of first- and second-order indices

According to the mathematical theory, the sum of all sensitivity indices of the first and all higher orders is equal to 1. In order to assess the RS-HDMR results we calculated the sum of all first- and second-order sensitivity indices. The time-dependent curves are presented in Fig. 2.27 for sample sizes between 512 and 16 384. The lowest number of runs is obviously insufficient for both models, as the resulting sum is far above 1. This is even more pronounced in the case of the LILW7 model, where the sum reaches values up to 3.6. Generally, the number of runs needed for reliable sensitivity analysis increases with the number of varied parameters, so this result is understandable.

For all sample sizes of 1 024 or more the sum curves of both models remain below 1, which is mathematically consistent. The curves for sample sizes above 2 048 practically agree with each other, except for times below 30 000 years. During this time, the sum of SI1 and SI2 is relatively low, which is a sign of existence of relevant higher-order interactions. For both models, the curves for 8 192 and 16 384 runs are nearly identical.

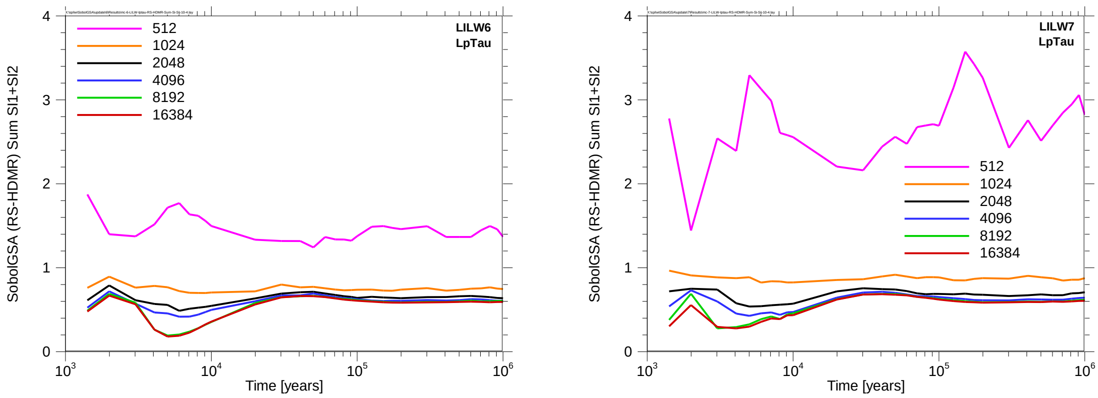


Fig. 2.27 Sum of sensitivity indices of the first (SI1) and second order (SI2) of the LILW6 and LILW7 models obtained by the RS-HDMR approach with different numbers of simulations

2.5.2.1.4 Conclusions

It was shown that the RS-HDMR meta-modelling approach as provided in the Sobol-GSA software is capable of computing Sobol' sensitivity indices of the first, second and total orders with relatively low computational efforts. The method was applied to the highly nonlinear and partly discontinuous LILW repository model.

The obtained RS-HDMR-results for the first-order indices were compared with those calculated with the EASI and SDP methods. The following conclusions were made:

- All three methods agree well with sample sizes of more than 1 000 points.
- With more than 2 000 simulations smooth curves are obtained.

- SobolGSA (RS-HDMR) and EASI required similar evaluation times, which were below 30 seconds for 31 points in time. SDP needed at least 94 % more evaluation time for the LILW6 model compared to SobolGSA (RS-HDMR) and EASI.

The second- and total-order indices could only be calculated using the RS-HDMR approach. As the classical Sobol' method and the EFAST method basically failed with the LILW models in former investigations, there is no possibility to verify the results. Nevertheless, the results can be assessed for mathematical consistency and plausibility:

- All calculated indices are mathematically valid (between 0 and 1).
- The sum of all first- and second-order indices is below 1.
- The results are physically plausible and agree qualitatively with the expectations based on the understanding of the system.

The investigations presented are neither a proof of validity of the RS-HDMR approach nor a verification of the SobolGSA software, at least as the second- and total-order indices are concerned. Nevertheless, they show the applicability of the approach and the software to a complex, highly nonlinear and discontinuous model that had, in former investigations, led to failure of other sensitivity analysis methods like EFAST or the classical Sobol' approach. RS-HDMR is the only available method that allows calculation of the second- and total-order sensitivity indices of this system, producing stable and at least plausible results.

2.5.2.2 Sensitivity analysis benchmarking

In several countries, systematic sensitivity analysis has been considered an essential part of the repository performance assessment process for a long time. The approaches and methods applied, however, are quite different and do not provide all the same information about the model under investigation. For a number of years, an exchange of experience on this subject has taken place between German and US groups. Other European organisations expressed their interest in participating in this cooperation.

In order to allow a better assessment of approaches, methods and tools, it is planned to execute a benchmarking exercise with a number of model systems of different complexity, oriented at different national programmes. This exercise is expected to yield a deeper understanding of what the modeller can learn from different types of sensitivity analysis and which types are best appropriate for which kind of model. Groups from five organisations from four countries have agreed to start this benchmarking exercise. These are:

- Sandia National Labs, USA,
- GRS, Germany,
- TU Clausthal, Germany,
- SCK*CEN, Belgium,
- Posiva, Finland.

As a first step, six model systems were selected, for all of which probabilistic calculations already exist or are planned to be done in the near future. These results are shared among the participants, and each group analyses them with their own methods and tools.

2.5.2.2.1 The model systems

In the following, the six model systems together with their input and output are shortly described[2].

HLW/SF repository in clay (GRS)

General description

This model system describes a generic repository for high-level waste and spent fuel in a Northern German clay formation. It is based on considerations made in the context of former projects on clay repositories. The repository is assumed to be located in the middle of the Apt layer in the Lower Cretaceous Clay in Lower Saxony. The model comprises the near field with the waste containers, three clay layers (bentonite buffer, Apt and Alb) and the biosphere. The radionuclide mobilisation and the (purely diffusive) transport through the clay layers were calculated with the near field code CLAYPOS, the far field with the code module CHETLIN and for the biosphere the code module EXMAS was used.

[2] Descriptions were partially provided by the relevant organizations.

Input

Number of input parameters: 6. All input parameters are scalar values and represented by continuous variables. One parameter is distributed uniformly, the others have log-uniform distributions. Several sets of calculations are available, made with Random, LHS, EFAST, RBD and quasirandom LpTau samples of sizes between 4 096 and 16 384. All parameters are independent, statistical parameter dependencies were not taken into account. All parameter uncertainties are considered epistemic and treated in the same way.

Output

The model output is the annual dose to a human individual, calculated as a series in time (194 points in time).

Known particularities of model behaviour

None, the model behaves smoothly.

SNF repository in shale (SNL)

General Description

The model describes a generic repository for commercial spent nuclear fuel in a shale host rock. Over the million-year simulation, the repository is undisturbed – no disruptive geological events and no human intrusion. The near field and far field are simulated in a single 3-D model domain, containing layered stratigraphy, the repository, and a household well (a simple biosphere) downgradient of the repository. The repository is in a thick, low permeability shale with higher permeability aquifers above and below the shale. It holds thousands of waste packages, each of which is a heat and radionuclide source. A waste package radionuclide source term is activated at the time of waste package breach (which depends on temperature and a sampled waste package degradation rate constant). Radionuclide transport away from the repository is primarily diffusive until radionuclides reach the aquifers, when advection driven by an applied pressure gradient becomes important. The model is described in /MAR 17/.

Input

Number of parameters: 10. All input parameters are scalar values and represented by continuous variables. Log-uniform and uniform distributions were used. Latin Hypercube Sampling (LHS) was utilised, sets of 50 and 200 runs are available. All parameters are independent, statistical parameter dependencies were not taken into account. All uncertainties are epistemic.

Output

The conducted UQ/SA analyses consider maximum concentration and dose over time at particular points in space.

Known particularities of model behaviour

None.

Dessel surface LILW repository (SCK·CEN)

General Description

This numerical model has been used for the safety analysis of the category A waste (LILW-SL) disposal facility as planned by ONDRAF/NIRAS for the Dessel site in Belgium. The radionuclide release from a concrete storage facility is modelled in which the complex interplay between matrix diffusion, flow and transport in fractures and porous media makes up for an interesting case study for a sensitivity analysis. Another interesting aspect is the switch from a diffusion-dominated system into an advective regime at a given time.

The sensitivity of the model and the uncertainty on the output can be investigated for three typical radionuclides with a distinct migration behaviour in concrete: the poorly sorbing ^{129}I, the moderately strong sorbing ^{59}Ni and the very strongly sorbing ^{239}Pu.

The calculations have not yet been done. A comparable sensitivity analysis was performed on the PA models used for the license application file submitted in 2013, with at that time slightly different conceptualisations in terms of radionuclide transport and timescales. This will be reported in /GOV 18/.

Input

Number of parameters: ~20. Most parameters are scalar, waterflow and K_d-values (in certain regions) will change at a given point in time. Different material-dependent values in the different domains. All parameters are continuous. Parameter dependencies are not taken into account. Uniform and log-uniform (with ranges up to 2 orders of magnitudes) distributions are utilised. Latin Hypercube Sampling (LHS) is utilised, 1000 runs per radionuclide are planned.

Output

The model calculates fluxes between compartments and the release from the facility (annual dose).

Known particularities of model behaviour

Proven non-monotonicity of diffusion coefficient, fracture flow, switch from diffusive to advective system.

LILW repository in rock salt (GRS)

General Description

The model describes a hypothetical repository for low- and intermediate-level radioactive waste (LILW) installed in an abandoned salt and potash production mine in a salt formation. It is oriented at the existing Morsleben repository and reflects its main particularities. The system consists of two emplacement areas, a large mine opening without waste and a small void in the center acting as a mixing tank. The emplacement area that contains most of the radioactive inventory is separated from the rest of the mine by a seal that is subject to chemical corrosion and loses its integrity after some time, depending on different parameters. The unsealed part of the mine is assumed to be filled with brine immediately after some time, then brine starts percolating through the seal. Salt creep and gas production lead to convergence of voids, fluid movement and radionuclide transport. The contaminant outflow from the mine was calculated using the code LOPOS, followed by a 1D far field path and a standard biosphere. The model is documented in /SPI 17/.

Input

Number of input parameters: 20. Calculations also exist for subsets with 6, 7 and 11 parameters. All input parameters are scalar values and represented by continuous variables. Uniform, log-uniform, log-normal and triangular pdfs have been used. All parameters are independent, statistical parameter dependencies were not taken into account. Sets of calculations are available for random, LHS, EFAST, RBD and quasirandom LpTau samples and different sample sizes between 3 000 and 32 790. All parameter uncertainties are considered epistemic and treated in the same way.

Output

The model output is the annual dose to a human individual, calculated as a series in time (301 points in time).

Known particularities of model behaviour

The model is highly nonlinear. Seal failure arises nearly suddenly after some time, depending on parameter values, and causes a considerable change in model behaviour, normally including a sudden increase of the output value that looks quasi discontinuous. One parameter (gas entry pressure) acts like a discrete parameter as it is practically only relevant if the value is below or above the threshold of 1.0 MPa. Several parameters have a non-monotonic influence or change their direction of influence over time.

SNL reactive transport model

General Description

The Fuel Matrix Degradation Model (FMDM) is a 1D chemical reactive transport code that has been coupled with PFLOTRAN. Its purpose is to calculate the waste form degradation rate ($g/m^2/yr$). However, it runs too slowly for a 3D repository simulation with thousands of waste packages. The objective of this candidate example is to develop a fast and accurate meta/surrogate model from a pre-processed multidimensional response surface.

Input

Number of input parameters: ~13. All parameters are scalar, but two are a pre-determined function of time (temperature and dose rate) or some are outputs from the previous time step (chemical concentrations). All parameters are continuous. Initial values of chemical concentration parameters (UO_2^{2+}, $UO_2(CO_3)_2^{2-}$, UO_2(aq), H_2, O_2, H_2O_2, CO_3^{2-}, and Fe^{2+}) may be sampled from somewhat large distributions. Precipitate amounts (U(IV)(s), U(VI)(s)) are initially zero but may increase with time. Dose rate at the surface over time, fuel burnup, and temperature are important input parameters. Sampling methods and number of runs have not yet been established but runs will attempt to cover the likely relevant sample space in a fairly systematic way so that a good response surface can be defined.

Output

There is just one scalar output at each time step: the fuel degradation rate (g/m^2/yr).

Known particularities of model behaviour

None expected.

SNL crystalline case

General Description

The model describes a generic repository for commercial spent nuclear fuel in a crystalline host rock. Over the million-year simulation, the repository is undisturbed – no disruptive geological events and no human intrusion. The near field and far field are simulated in a single 3-D model domain, containing a stochastically generated heterogeneous permeability field representing fractured crystalline rock, a thin layer of sedimentary overburden, the repository, and an observation well downgradient of the repository. The repository holds thousands of waste packages, each of which is a heat and radionuclide source. A waste package radionuclide source term is activated at the time of waste package breach (which depends on temperature and a sampled waste package degradation rate constant). Radionuclide transport away from the repository is primarily advective (especially at early times when waste packages are hot) and is driven by both an applied regional pressure gradient and expansion and buoyancy of the water in the hot repository. The model is documented in /MAR 16/.

Input

Number of input parameters: 8 sampled scalar and continuous parameters plus the stochastically generated permeability field, which varies in space. All parameters are independent. Uniform and log uniform distributions are used. The 8 sampled parameters are epistemic. Latin Hypercube Sampling (LHS) is utilised. For the first step, 50 simulation runs are foreseen.

Output

UQ/SA analyses conducted to date consider maximum concentration at particular points in space.

Known particularities of model behaviour

The relationship between maximum concentration and input parameters is non-monotonic. Some combinations of parameters resulted in messy or exceptionally long runs.

2.5.2.2.2 Sensitivity analysis of the shale repository system

The benchmarking exercise will be done and documented in detail in the next phase of the project. Some orienting calculations were already performed by several organisations. In this chapter, the results achieved by GRS for the SNL shale repository system are presented. These results were obtained by applying some of the sensitivity analysis methods identified in /SPI 17/ to the available set of 50 calculation runs.

Model output results are available for two radionuclides (^{129}I, ^{237}Np) at 9 points in space. They represent the maximum radionuclide concentration over time. Tab. 2.4 lists the names and meanings of the model input parameters and output (response) functions.

Tab. 2.4 Parameters and output functions of the SNL shale repository model

Parameter name in report /MAR 17/	**Parameter name**	**Description (references refer to /MAR 17/)**
WP Degrad Rate	rateWP	Mean base waste package degradation rate used in the truncated log normal distribution that creates spatial variability – see Chapter 4.4.2.5
Shale ϕ	pShale	Porosity of the repository shale host rock – see Figure 4-5
SNF Degrad Rate	rateSNF	Fractional fuel matrix dissolution rate for spent nuclear fuel – see Chapter 4.4.2.5
U. Sand k	kSand	Permeability of the aquifer (sandstone) that sits on top of the shale host rock – see Figure 4-5
Limestone k	kLime	Permeability of the aquifer (limestone) that sits beneath the shale host rock – see Figure 4-5
L. Sand k	kLSand	Permeability of the aquifer (sandstone) that is sandwiched inside the lower shale – see Figure 4-5
Buffer k	kBuffer	Permeability of the bentonite buffer – see Figure 4-8
DRZ k	kDRZ	Permeability of the disturbed rock zone – see Figure 4-8
Shale Np Kd	sNpKd	Linear distribution coefficient for Np in the shale host rock
Buffer Np Kd	bNpKd	Linear distribution coefficient for Np in the bentonite buffer
Max [129I] at sand_obs1	sand_obs1	Max [129I] 30 m in upper sandstone – see Figure 4-20
Max [129I] at sand_obs2	sand_obs2	Max [129I] 2500 m in upper sandstone – see Figure 4-20
Max [129I] at sand_obs3	sand_obs3	Max [129I] 5000 m in upper sandstone – see Figure 4-20
Max [129I] at lime_obs1	lime_obs1	Max [129I] 30 m in limestone – see Figure 4-20
Max [129I] at lime_obs2	lime_obs2	Max [129I] 2500 m in limestone – see Figure 4-20
Max [129I] at lime_obs3	lime_obs3	Max [129I] 5000 m in limestone – see Figure 4-20
Not used in report	response_fn_7	Max [129I] 30 m in lower sandstone

Not used in report	response_fn_8	Max [129I] 2500 m in lower sandstone
Not used in report	response_fn_9	Max [129I] 5000 m in lower sandstone
Not used in report	response_fn_10	Max [237Np] 30 m in upper sandstone
Not used in report	response_fn_11	Max [237Np] 2500 m in upper sand-stone
Not used in report	response_fn_12	Max [237Np] 5000 m in upper sand-stone
Not used in report	response_fn_13	Max [237Np] 30 m in limestone
Not used in report	response_fn_14	Max [237Np] 2500 m in limestone
Not used in report	response_fn_15	Max [237Np] 5000 in limestone
Not used in report	response_fn_16	Max [237Np] 30 m in lower sandstone
Not used in report	response_fn_17	Max [237Np] 2500 m in lower sand-stone
Not used in report	response_fn_18	Max [237Np] 5000 m in lower sand-stone

Comparison of results

In /MAR 17/, Spearman's rank correlation coefficients were computed using the DAKOTA software /ADA 12/, /ADA 13/. These coefficients, among others, were re-calculated using the RepoSUN tool /BEC 16/ for the benchmark exercise. Fig. 2.28 shows the comparison of the results achieved by SNL and GRS for ^{129}I concentration at the upper sandstone and limestone observation points. The calculated values are nearly identical, except from those for observation point 3 in upper sandstone. In the latter case, small differences were found, which could not be explained so far, this requires deeper investigations of what the different programs do with the data. In principle, however, the tools confirm each other.

Sensitivity analysis with RepoSUN

For each set of model output values, seven sensitivity measures were calculated using the RepoSUN tool:

1. the Pearson correlation coefficient,
2. the Standardised Regression coefficient (SRC),
3. the Partial Correlation Coefficient (PCC),
4. the Spearman Rank correlation coefficient,
5. the Standardised Rank Regression Coefficient (SRRC)

6. the Partial Rank Correlation Coefficient (PRCC),
7. the first-order sensitivity index, using the EASI method.

The methods and their characteristics are explained in /SPI 17/.

Fig. 2.29 and Fig. 2.30 show the calculated sensitivity measures for the concentrations of ^{129}I and ^{237}Np at the six observation points in upper sandstone and limestone. Negative values indicate an inverse sensitivity (higher parameter value – lower model output value). As, however, the sensitivity index calculated with EASI is a variance-based measure, it is always positive. Interestingly, for some parameters of minor importance different measures seem to indicate different directions of influence. This is probably a consequence of the low number of simulations, which results in a low robustness and reliability of the sensitivity analysis results. Nevertheless, all methods are in general agreement about the most influential parameters.

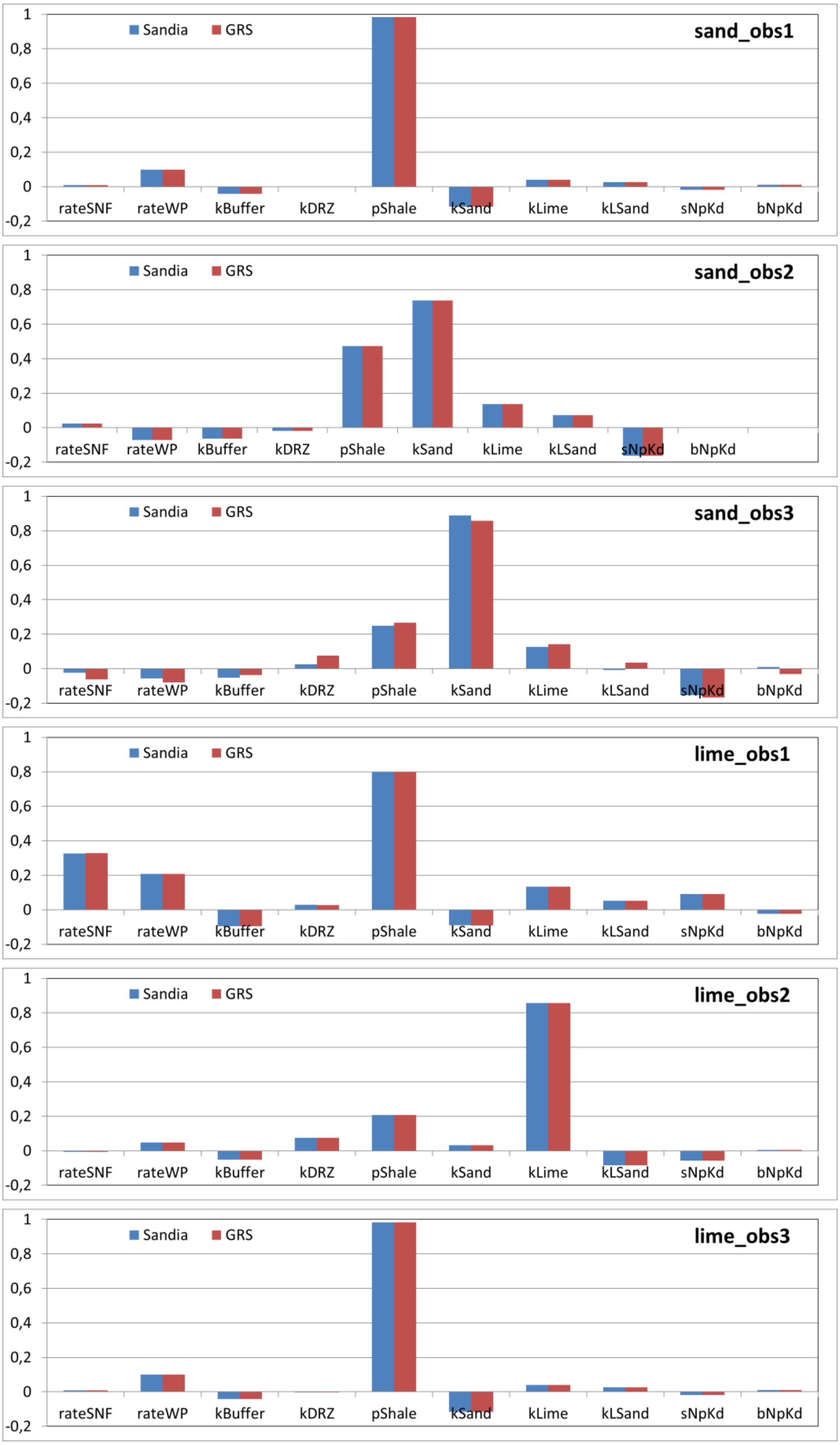


Fig. 2.28 Spearman rank correlation coefficients calculated by SNL and GRS

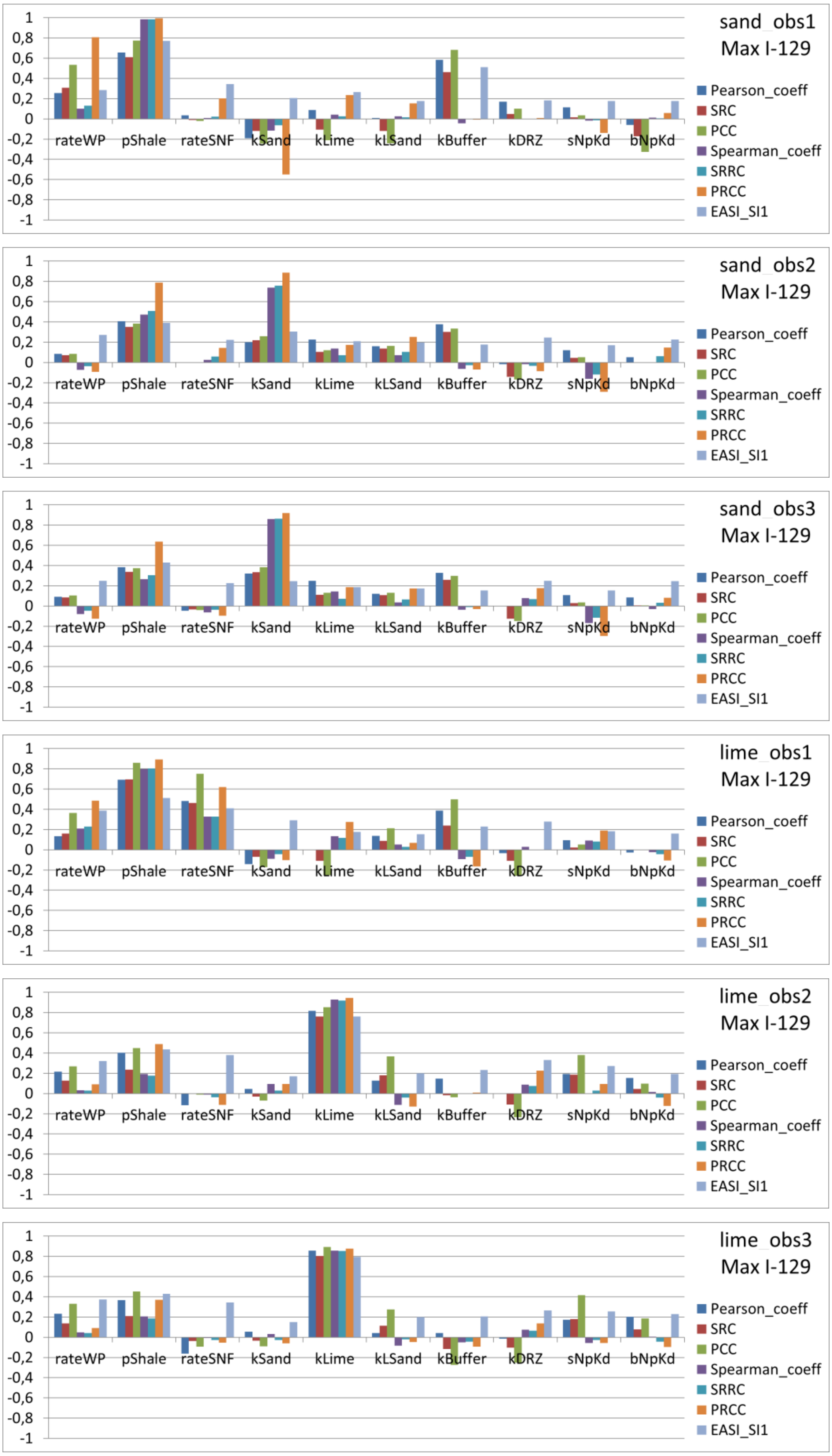


Fig. 2.29 Different sensitivity measures for ^{129}I at six observation points

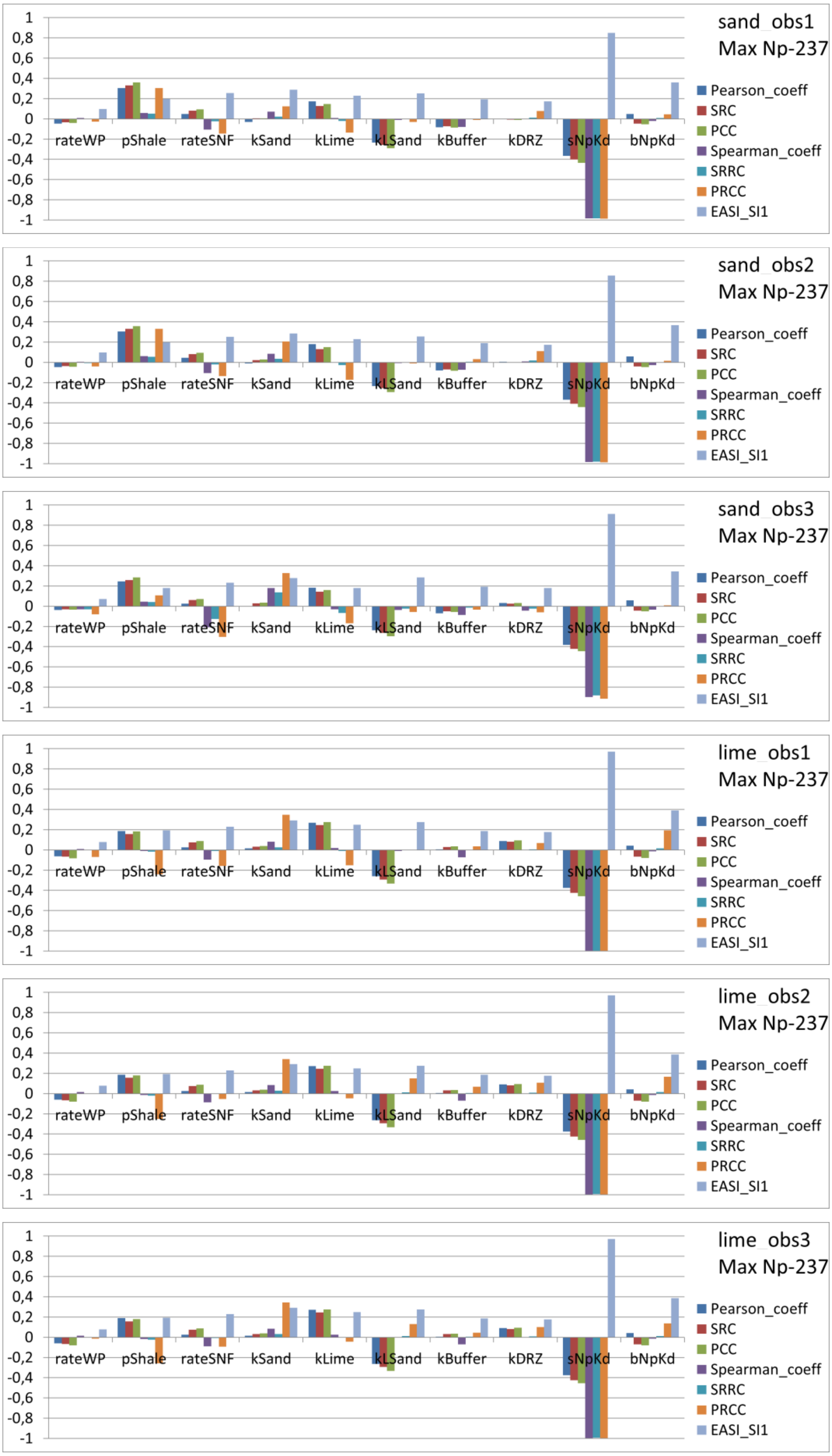


Fig. 2.30 Different sensitivity measures for ^{237}Np at six observation points

2.5.2.3 Conclusions and outlook

The orienting exercise presented here shows that the tools DAKOTA and RepoSUN calculate very similar rank correlation coefficients, which can be seen as a mutual verification of the tools. Even on the small basis of 50 model runs the leading sensitivities of the SNL shale repository model seem to be identified; this, however, needs further confirmation, based on a higher sample size. Moreover, the investigations with RepoSUN indicate that the different sensitivity measures more or less agree only for the one or two most sensitive parameters. This is most probably also due to the small sample size and should be interpreted as a hint that a significant sensitivity analysis is not possible with such a low number of model runs, at least for the less sensitive parameters. This, however, needs further systematic investigation. For the next phase of the sensitivity analysis benchmarking exercise, the following investigations are foreseen:

- analysis of the new set of 200 model runs, and maybe a set with even more runs, with the SNL shale repository model, using both DAKOTA and RepoSUN,
- application of further sensitivity analysis methods, e. g. graphical methods,
- estimation of statistical significance of sensitivity measures,
- analysis of the other model systems, according to availability of calculation results,
- comparison of sensitivity analysis results with those obtained by other organisations with their own tools,
- drawing conclusions concerning
    - significance of different methods,
    - sample sizes necessary for reliable sensitivity analysis,
    - influence of model complexity,
    - interpretation of sensitivity analysis in the context of different repository systems.

2.6 Communication aspects

The aspect of communicating the safety case is paid increasingly attention on national as well as on international level. Issues related to communication are currently also addressed by working groups of the NEA. Two activities have been strongly supported and are highlighted in this report, namely (i) communication of complex technical contents of the safety case to lay people (Chapter 2.6.1) and (ii) how to preserve records, knowledge and memories of a radioactive waste repository after its closure for future generations (Chapter 2.6.2).

2.6.1 Safety case communication

Compiling the safety case for a deep geological repository is a highly technical undertaking involving a number of scientific disciplines. The selection of materials and approaches used in designing a geological disposal facility involves availability, constructability and scientific considerations. The safety case also substantiates the myriad decisions that go into the design of a safe operating system and ensures that its long-term performance meets safety criteria and satisfies regulatory requirements. Compiling a safety case thus generates an extensive set of voluminous documents with technical and scientific content.

The documentation, observations and field and laboratory studies that support a repository safety case, as well as the analyses themselves, are likely to be both massive and unintelligible to a typical “stakeholder”, and more so to the average member of the public. Yet it is the stakeholders and the public that will be asked to accept that a proposed repository will be safe during its lifetime and long afterwards. The challenge is to communicate the case for safety in plain language – which accurately reflects the outcome of the many technical studies, analyses and calculations.

Based on this an IGSC working group on Safety Case Communication was created with the mandate to investigate the issue of communicating scientific information with non-technical stakeholders. This group conducted a literature review of communications related studies, and documents, particularly NEA technical documents and European Commission study technical documents. In addition, several IGSC member organisations were each asked to write their lessons learned from a recent major national communications activity. The main aim of this review was to synthesize effective communication approaches/strategies, as well as to improve understanding of communication difficulties and challenges.

The working group documented the result of its' work in the NEA report "Communication on the Safety Case for a Deep Geological Repository" /NEA 17/. The report describes general principles and objectives of stakeholder communications and to plan it in advance. The following elements should be addressed in communication planning:

- Define the scope and objectives for any given communications effort.
- Derive the central messages to be communicated.
- Identify target groups and tailor the messages for understanding technical subjects.
- Select communication channels and tools to deliver the information and key messages in an effective manner.
- Design instruments and practices, including shared platforms, that allow communications effectiveness to be achieved and measured.

In addition, the process of capacity building and awareness is discussed and how to deal with divergent views and ways to tailor the message. Local communities may lack of competences. Capacity building helps communities to understand complexity of RWM. It is recommended to provide platforms to promote networking of local communities – share and discuss experience and concerns, to learn from each other and form therewith stronger linkage.

General safety case communications aspects including definitions, the concept of a platform for dialogue, the role of peer reviews, regulatory aspects, materials and methods, and recommendations for presentation and dialogue are described in the report. Implementers and regulators should both be involved in stakeholder outreach and dialogue. Basic rules of civil dialogue and pointers for effective two-way communication are described. As shown through past failures and successes, communication is an interactive process and can be a complex and challenging task. When conveying complicated or technical information to the public in plain language, clear, accurate and accessible information that does not minimise or exaggerate issues has been found to be necessary and practical. In addition, a more detailed and in-depth discussion of the major points to be discussed in order to convey a safety case, namely fundamental issues of a safety case, monitoring, retrievability, indicators and natural analogues is outlined in the report.

Communication clearly has a specific role in repository development. Through effective communication among stakeholders, technical experts are able to hone their communication skills and communication experts are effectively integrated into the development process. An essential starting point for all such communication is trust in the communicator. Therefore, building trust with stakeholders, especially the local community, is the key requisite for effective communication with the public.

The purpose of the work was to collate the lessons learnt and insights from that collective experience to guide ongoing stakeholder communications efforts by implementer and regulators. Based on the report a co-operation with the Forum of Stakeholder Confidence (FSC) on communication of the safety case was started. This FSC consist amongst others of communication experts and has long experience in addressing the challenges associated with societal issues related to radioactive waste management and stakeholder engagement. As a first step a joint IGSC/FSC workshop on collaboration between IGSC/FSC – safety case communication was held in September 2017. Several topics of potential co-operation between both groups were identified. Currently these topics are prioritized, and specific cooperation projects are being planned.

2.6.2 The Preservation of Records, Knowledge & Memory Across Generations (RK&M)

GRS has participated in the NEA initiative “The Preservation of Records, Knowledge & Memory Across Generations (RK&M)” /NEA 18a/. The objective of the RK&M initiative was the development and publication of a ‘menu’ of approaches and mechanisms to preserve RK&M about radioactive waste disposal facilities /NEA 18a/. National disposal programmes can then select components from this menu to create a system that maximises the likelihood of information survivability while meeting the legal requirements in force. This is referred to as a ‘systemic strategy’ wherein a variety of avenues are established in order to maximize the likelihood that information survives and can be understood over the relevant timescale.

The menu contains a set of approaches including: memory institutions; time capsules; markers; culture, education and art; oversight provisions; international mechanisms; regulatory framework; knowledge management; and dedicated record sets and summary files. Each approach is composed from mechanisms for which unique descriptions have been developed based on a standard template /NEA 18a/. The list of approaches and its identified mechanisms are shown in Tab. 2.5.

Tab. 2.5 Approaches and their corresponding mechanisms developed in /NEA 18c/

Approaches	**Mechanisms**
Memory institutions	Archives, libraries and museums
Time capsules	Large visible time capsules, large invisible time capsules and small time capsules
Markers	Sub-surface markers, surface markers, deep geological markers, surface traces and monuments
Culture, education and art	Surface infrastructure as industrial heritage in itself; alternative reuse of the site and/or its infrastructure; heritage inventories and catalogues; local history; intangible cultural heritage; nuclear and related topics in (academic) education, research and training; information dissemination activities; and nuclear and related topics in art
Oversight provisions	Monitoring, land use control and clear and planned responsibilities
International mechanisms	International treaties, conventions and directives; international standards and guidelines; international inventories and catalogues; international cooperation; and international education and training programmes
Regulatory framework	National regulatory framework and safeguards
Knowledge management	Knowledge retention tools, knowledge risk analysis and knowledge sharing philosophy
Dedicated record sets and summary files	SER and KIF

With respect to the safety case particularly important components of a RK&M preservation strategy are the KIF and the SER. A KIF (Key Information File, /NEA 18b/) is designed to be a single, short document, produced to a standard format, aimed to allow society to understand the intent of the repository, and thus to reduce the likelihood of unnecessary human intrusion. The KIF is proposed to be openly available and ultimately widely distributed. Three tests on national KIF documents as examples, were performed by France, Sweden and the USA. A summary of those can also be found in /NEA 18b/.

Most effort from this project was provided for the SER (Set of Essential Records, /NEA 18c/). The SER can be understood as a collection of the most important records for waste disposal selected for permanent preservation during the repository lifetime. It provides sufficient information for current and future generations to ensure an adequate understanding of the repository system and its performance. This will enable them to review and verify the repository performance and the safety case and to make informed decisions.

During repository implementation, construction, operation and closure, a large number of records that are diverse in nature (e. g. paper documents, engineering drawings, maps, photographs, physical objects or electronic records) will be produced. In order to keep the information preserved for future generations clear, transparent and traceable, the RK&M initiative developed an example procedure to identify a reduced set of records. The proposed procedure is based on the representative needs of future generations related to the repository and on a classification and rating scheme applied to all of the records produced during the lifetime of the repository. The proposed classification and rating scheme comprises two aspects. The relevance of the respective record for the formulated need of the future generation and an estimation of the effort it would take for a future generation to re-create the information contained in the record (i. e. if record transfer from the past had failed).

The pre-operational and operational phases of the repository will last over many decades. It is strongly recommended to start the SER selection process as early as possible in the repository programme to avoid the risk of loss of important information that might not be available at a later stage. Although it is likely that regulations will require one organisation, possibly the implementer, to be responsible for the selection and compilation of the SER, the large variety of records suggests that multi-disciplinary teams should be involved.

It is clear that the development of the SER will be an ongoing process that should be under continuous maintenance and be regularly reviewed before repository closure. These reviews might be connected with regular updates of the safety case or other activities required by regulations.

Since the final SER in its final state will contain numerous records, only one version should be created existing in at least two copies. To allow future generations to easily and efficiently discover the information, search tools based on international archival description standards should be part of the SER. Meta information can be added to each record for better understandability.

With respect to the preservation of the SER during the repository lifetime, electronic media have the advantages of providing high data storage, easy searching and multiple copies. However, such media are not recommended for the long-term preservation due to their relatively low durability and the need for permanent maintenance, updates or upgrades of hardware and software tools. At the time of the study presented, permanent paper seems to be the best option. However, this decision should be taken by archiving specialists at the time that the SER is finalised.

The proposed procedure for SER selection has been illustrated by examples of records compiled using information regarding record creation and preservation from the near surface repositories El Cabril in Spain and La Manche in France. As a next step, the procedure should be applied in order to evaluate its feasibility and identify any shortcomings. A second recommendation is required to further evaluate the review process for compiling the SER. The proposed classification and rating scheme can be part of the review process, but other instruments might be identified and applied.

3 International developments and co-operation

As an important part of the project international developments are followed and national research results are presented to the international community. In this respect, the participation in working groups of the OECD/NEA and IAEA plays a central role.

3.1 RWMC

The Radioactive Waste Management Committee (RWMC) of OECD/NEA was created in 1975. Ever since it provides a forum of senior representatives from regulatory authorities, radioactive waste management and decommissioning organisations, policy making bodies, and research-and-development institutions from the NEA member countries. The International Atomic Energy Agency (IAEA) participates in the work of the RWMC, and the European Commission (EC) is a full member of the Committee. The RWMC aims at assisting member countries in developing safe, long-term management of radioactive waste while continuing to support adaptive radioactive waste management plans in response to evolving societal expectations and values and changes in public policies. In 2017 Romania and Argentina joined the OECD/NEA, so that, overall, the NEA has now 33 member countries.

In 2015 discussions started within NEA's RWMC how the future Programme of Work should be structured in order to reflect the common radioactive waste management requirements of member countries at both national and multi-national levels. In 2017 a RWMC Statement was discussed and finalized, the purpose of which was to identify the needs of RWMC member countries and to guide the development of the RWMC's future activities in a systematic manner using a holistic, sustainable approach to manage radioactive waste. In particular, the RWMC statement presents a methodology for transforming the vision of the RWMC into tangible work activities.

The concept of sustainable development essentially comprises three constituents: (1) environment, wherein radioactive waste management should demonstrate safety through science and technology; (2) economics, in which sufficient funding and cost optimisation should be assured; and (3) society, where ethical aspects as well as social trust and confidence are built into all activities of waste management. These three constituents are applicable to the overall radioactive waste management process from generation to disposal or in other words "from cradle to grave" (see Fig. 3.1). It is also envisaged that the radioactive waste management system must be embedded in national legislative, regulatory and organizational frameworks. These frameworks, which can vary significantly from country to country, are in place to provide a basis for RWM activities in each of the stages in the waste management path.

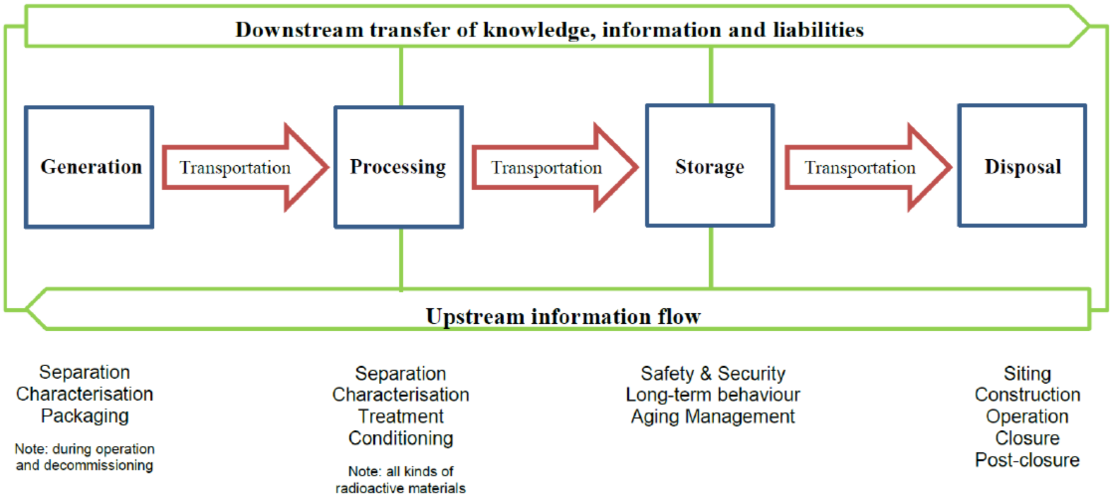


Fig. 3.1 The overall radioactive waste management path from generation to disposal of waste, acknowledging the inclusion of regulatory and licensing processes as well as safe operation

The radioactive waste pathway, as depicted in Fig. 3.1, entails a comprehensive transfer of knowledge, information and liabilities from generation to disposal of waste. In the same manner, new knowledge / information gained at each stage in the path serve to inform decisions of the previous stages, i. e. upstream flow of information. For example, waste acceptance criteria for disposal will inform the suitability of storage practices, whilst waste storage requirements may influence processing methods and generation procedure. In developing these stages, key elements such as infrastructure and materials management, safety and security, monitoring, funding and licensing, procedural ownership and liabilities and sustainability, should be considered.

Subsidiary bodies, under the guidance of the RWMC, carry out focused work to support the RMWC in achieving its goals. Relating to the adopted holistic, sustainable approach for establishing the future work programme discussions started how to organize the subsidiary bodies under the guidance of the RWMC.

In mid-2017, the NEA began creating a new standing technical committee on Decommissioning of Nuclear Installations and Legacy Management (CDLM) to bring together all decommissioning work into one stand-alone committee. It is planned that the Working Party on Decommissioning & Dismantling (WPDD) and its sub-groups will be transferred from the RWMC to the future CDLM. In 2018, the Steering Committee of NEA approved the creation of the CDLM as a new standing technical committee of NEA's RWM division and subsequently the revised mandates of the RWMC and the CRPPH. A kick-off meeting in planned for October (or November) 2018 to finalize CDLM's mandate and discuss the 1st draft of its Programme of Work. The first meeting of CDLM shall be carried out in early 2019 if timing allows.

The NEA secretariat presented a proposal for future work activities of the RWMC at the 51^{st} session of RWMC in April 2018. These proposals regard some substantial changes in scope and structure of subsidiary bodies under the guidance of the RWMC. They pertain to, for example, the scope of the IGSC work and the future organization of the work addressing information management issues, such as the Preservation of Records, Knowledge and Memory across Generations (RK&M), the Radioactive Waste Repository Metadata Management (RepMet) and the Expert Group on inventorying & reporting method (EGIRM). The secretariat's proposals are still discussed between the member countries and respective decisions will be taken at the 52^{nd} session of RWMC in 2019.

3.2 IGSC

GRS is actively participating in the work of the Integration Group for the Safety Case (IGSC). For the duration of this project important contributions to the IGSC work were presentations or chairing of topical sessions, coordination of the working group on Safety Case Communication (see Chapter 2.6.1) and participation in the IGSC core group, which is responsible for coordinating and steering IGSC work.

From the topical session "Relevance of gases in the post-closure Safety Case" and a review of IGSC of the FORGE project resulted an IGSC position paper on gases in the repository, which is described in Chapter 2.4.The results of the working group for safety case communication are described in Chapter 2.6.1.

Key results from the topical sessions (i) on extreme geological events, (ii) on the role of geoscientific arguments in the siting process, and (iii) on criticality and safeguards in deep geological repositories are described in the following sub-sections.

3.2.1 Siting

The topical session was an exchange of experiences from the siting process, as performed, or planned to be performed, in the different member countries of the IGSC. The focus was on the role and use of geoscientific arguments within the whole siting process. In particular, the objectives were to: (i) explore how members are planning or have used geoscientific arguments to identify suitable sites for geological disposal facilities; (ii) compile what geoscientific safety arguments have been used or are planned for use; (iii) explore how particular geoscientific safety arguments were received by stakeholders (both technical and non-technical) in countries where the siting process is advanced; and (iv) evaluate regulatory views / experience on using geoscientific safety arguments for siting.

The following presentations were given and can be found at https://www.oecd-nea.org/download/igsc/igsc-17/index.html.:

- The role of the geology in site selection in the US. Abraham Van Luik, Carlsbad Field Office, US Department of Energy
- Nomination of scientifically suitable areas within the revised site selection process in Japan. Hiroyushi Ueda, NUMO, Japan
- The UK national geological screening exercise. Glenda Crockett, RWM, UK
- Geoscientific arguments in the early stage of siting. Sona Konopásková, SURAO, Czech Republic
- The Use of Geoscience Data in the Early Phases of Canada's Siting Program for a Used Fuel DGR. Ben Belfadel, NWMO, Canada
- The new siting procedure in Germany and the role of geoscientific information. Jürgen Wollrath, BfS, Germany
- Geosciences within the siting process: the French experience. Emilia Huret and Guillaume Pépin, Andra, France
- Role of geoscientific arguments in the on-going siting process in Switzerland. Jürg Schneider, Nagra, Switzerland
- Using geoscientific argumentation for the siting process and in the construction licensing phase– experiences from Finland. Barbara Pastina, Posiva, Finland

- Role of geoscientific arguments in siting an SNF repository in Sweden. Allan Hedin, SKB, Sweden

3.2.1.1 Regulatory aspects

In some countries the siting process is very clearly described, e. g. in Switzerland. In the Sectoral Plan for Deep Geological Repositories a three-stage process is formulated, and the regulator prescribes in detail the calculation endpoints, namely the indicators to be calculated and used for each stage. The whole process is strongly based on geoscientific arguments.

The regulatory requirements on the use of geoscientific arguments in the siting process or generally in a safety case differ for each country. Some national regulations explicitly formulate high-level geoscientific requirements, as was for example the case of the Final Disposal Act in Japan. In Germany, the Working Group on a Site Selection Procedure for Repository Sites, AK-End, proposed to apply exclusion criteria, minimum requirements and weighting criteria derived from requirements for a favourable overall geological setting. However, the regulations in both countries are currently under revision and these requirements are not in force.

In other national regulations, for example in Sweden, no specific emphasis is placed on geoscientific arguments, but rather the focus is on the functioning of the whole system. In the US the disposal system is required to have at least one natural and one engineered barrier, but there are no natural subsystem requirements stated in current US regulations. In the UK the national policy was revised in 2014, setting out a Government-led staged process, in which information on geology is provided early in the siting process to assist stakeholder consultation.

Most national regulations, however, do not specify which geological arguments are to be considered in safety cases. Rather, it is left to the implementer to ensure that the safety case is sufficiently comprehensive, taking into account all relevant geoscientific data.

3.2.1.2 General aspects of the site selection process

In nearly all programmes the site selection procedure is a multi-stage process, which roughly consists of (i) an initial study, consisting of desktop work with a comprehensive literature/data survey, (ii) a second step with preliminary site investigations such as geophysical surveys and a limited number of boreholes and (iii) detailed investigations including, e. g. airborne surveys, further boreholes, excavation of test tunnels, or construction of and research in underground research laboratories (URLs). The siting process starts with a higher number of sites and during each step the number of sites taken forward is narrowed down. The detailed investigation step needs extensive and costly work and is typically carried out only for a maximum of one or two sites.

In the first step it was stated (e. g. in Japan) that literature/datasets need to be (i) quality assured in terms of credibility, (ii) publicly available in terms of transparency/traceability and (iii) be nationwide to avoid regional inequality. For example, in France data from previous exploratory wells for oil and gas industry were used, and previous seismic profile data were re-interpreted. At the second step with a preliminary site investigation, geological surveys, 2D seismic profiles and a selected number of boreholes may be used to identify global properties of potential host rock, such as thickness, permeability or diffusibility (e. g. Andra). Subsequently, a more detailed site investigation with e. g. 3D seismic surveys, high resolution airborne surveys, additional and maybe deeper boreholes, and investigations in URLs and laboratories would greatly increase the geoscientific knowledge and form the basis for the application of THMC models and comprehensive safety assessments. These are rough commonalities and might vary to some extent for each national programme.

Differences concerning the abundance of host rock types in different countries have an impact on how the siting process is shaped and criteria are applied. For example, crystalline rock, rock salt, and sedimentary clays and clayey shales are all available in the USA. In the case of WIPP the choice of the host rock was the product of a general recommendation for the use of salt rock by the National Academy of Sciences. The general location of the WIPP site was selected based on previous exploratory work in and around the Delaware basin. The choice of the specific site was then the product of the subsequent volunteering of the town of Carlsbad and based on drilling for site characterization and the features found. In the case of Sweden and Finland, where clay or salt sites are not available, crystalline sites were studied and geoscientific arguments were developed specifically for this rock type. As such, relatively many sites could be considered potentially suitable at the beginning of siting. Thus, both geoscientific arguments and acceptance by the local community were sought at different stages of the siting process.

The role of voluntarism in the siting process and the stage of the process in which voluntarism – if any – comes into play differ widely. In several countries voluntarism plays a key role, e. g. local acceptance is a prerequisite in both the Swedish and UK siting processes. Another example of voluntarism in the early stages of siting is the 'Adaptive Phased Management approach', as applied in Canada, where technical and social aspects are advanced in parallel to find an informed and willing community.

In some other countries no voluntarism at all is foreseen in the siting process. In the Czech Republic a voluntarism approach failed, and the responsibility was shifted from the municipalities back to the government. In Switzerland, the 'Sectoral Plan' is being conducted to identify the most suitable site, with local communities then being consulted regarding the implementation. In Japan and Germany, the role of socio-economic aspects in the siting process are currently being discussed intensively as the siting process in these countries is under revision.

3.2.1.3 Evaluation factors and criteria

Several countries stated that geoscientific arguments played a key role in the siting process. Frequently, geoscientific arguments flow into criteria or evaluation factors, which are used to control the individual steps of the siting procedure. Such criteria might be exclusion criteria, minimum requirements, or criteria used for ranking. In Japan, three kinds of classifications were discussed, namely areas to be avoided, areas to be preferably avoided and preferable areas. Typical exclusion criteria concern the occurrence of large area vertical movements or active fault zones in the area. The use of such criteria is however dependent on the geological situation in each country. For example, the Japanese programme cannot avoid operating within tectonically active regions and showing that extreme geological events will not compromise repository safety is thus an essential component of the safety case. The Japanese programme has therefore developed advanced methods for the identification of volcanic and tectonic hazards at potential repository sites in Japan in terms of their likelihood and scale, which can provide a basis for site comparison (cf. Topical Session of extreme geological events, IGSC-16).

Many countries formulated minimum requirements, which have to be fulfilled, e. g. a 100 m thick host rock, a minimum and maximum depth of 300 m and 1 500 m, respectively, as for example proposed by the German Working Group AK-End. Nearly all countries formulated arguments as a prerequisite that any suitable site must ultimately satisfy. The following are frequently regarded as attributes of a stable geological system:

- low seismicity,
- low earthquake, fault, and igneous activities,
- low uplift and erosion rates,
- no occurrence of unconsolidated Quaternary deposits.

During the discussion it was mentioned that it is important not only to consider the current situation, but to evaluate these aspects for the whole assessment time frame. A system which is considered stable today, might evolve in the future to a less stable system, e. g. seismic events or uplift rates might significantly increase in the future. A second group of attributes concerns favourable properties in the host rock, formulated as:

- low permeability or low groundwater flow in the host rock,
- favourable rock-mechanical conditions,
- good thermal and mechanical properties,
- favourable geochemical properties to limit radionuclide migration.

The role of each individual attribute is, of course, to some extent dependent on the host formation. A general agreement was observed in the robustness of the geoscientific safety arguments related to these attributes. In this context the ease of characterisation, the homogeneity and predictability were emphasised.

It is a current trend that these arguments are directly related to safety functions, for example containment, isolation and retention. In some countries the arguments for the geological formation on its own are most relevant, e. g. in the UK, where a guidance has been developed on proposals to present geological information in an accessible form to stakeholders. In other countries, the arguments are embedded in the view on the whole repository system. In this context additional safety functions such as protection of the engineered barrier system (EBS) or criteria such as engineering suitability or stability were mentioned.

Some differences also exist in the role of other than geoscientific factors. In Finland in the step “Selection of the Preliminary Investigation Areas” further comparisons of the proposed sites were based also on other environmental factors, including population density, transport infrastructure, land ownership, protected areas and national resources. In addition, in Japan, for example, so-called 'nomination factors' for scientifically suitable areas under discussion, include pre-closure safety and the safety of the waste transport. Similarly, in the Canadian approach the safe construction, operation and closure of the repository as well as safe and secure transportation were included as two of six safety functions, which have to be fulfilled by any suitable site during the geoscientific site evaluation process.

Although there is agreement that water resource areas should be avoided, there are different views with regard to areas with mineral resources which might play a role with regard to past and present uses (resulting e. g. in avoiding locations of existing deep mines or of intensely deep-drilled areas), but also considering potential future uses. In some countries, absence of potential mineral resources represents an important argument in the site selection, whereas in others this argument does not play a role. This is particularly the case for countries that intend to use rock salt as the host formation, which is at least today an important mineral resource. Also, salt formations might function as a trap for hydrocarbons, a fact which might encourage investigation drillings even in the factual absence of such hydrocarbons. On the other hand, it is hard to tell which minerals will indeed represent a resource for future generations or which other site features (e. g. geothermal heat extraction, storage of hydrocarbons) might be of interest to future generations. The consequences of human activities, such as exploitation of the mineral, need to be evaluated and addressed in the safety case. In addition, the repository concept might be optimised to reduce potential consequences of future human actions. It was also mentioned that credit is taken from the NEA project "Preservation of Records, Knowledge and Memory (RK&M) across Generations", which evaluates ways to keep oversight of the repository as long as possible to minimise inadvertent human action, e. g. /NEA 13/.

3.2.1.4 Role of geoscientific information in different stages of the repository programme

As the repository programme evolves the (geoscientific) knowledge increases. Challenges in the early phase of the process are due to a limited availability of data and therewith large differences might exist in the resolution of data for different areas. In this case a workable approach might be the restriction to a subset of data, where a comparable range of information is available (cf. the Canadian approach). It is recommended to avoid defining criteria too early and / or too strictly in the process, prior to at least some substantial geoscientific knowledge being available. On the other hand, if criteria are defined in a late stage of the process, which increases flexibility, it might be perceived that requirements are tailored to the needs of the implementer, rather than being scientifically based. Further it was mentioned that in the early phase the use of verbal arguments is more valuable than quantitative comparisons. Uncertainties need to be acknowledged and appropriately accounted for when making comparisons. In a generic state, prior to site characterisation it is difficult to use safety assessment results for discrimination between sites, because it is likely to be just discrimination between assumptions.

In the early stage a generic safety assessment, however, can be useful for developing system and process understanding and identifying where further work is needed, but should not be applied for numerical comparisons. There is a need to manage the expectations for preliminary safety assessments and to explain to the stakeholders that these are not full safety cases and are likely to be based on qualitative or semi-quantitative arguments. Nevertheless, generic safety cases can give local communities and regulators confidence in the implementer's ability to make a safety case. Safety needs to be considered from the very start of the process. It is what stakeholders want to know about, but it will be assessed in different ways at different stages.

In this context the importance of a stepwise approach was mentioned, to narrow down siting regions until a full site characterisation is possible. Such an effort can only be performed for a limited number of sites and a detailed set of site data is the basis for a comprehensive safety case. So, in general, as the programme moves forward data and knowledge will increase and therewith confidence in modelling and results, i. e. geoscientific indicators become more meaningful. In this process the dialogue between implementer and regulator is seen to be important to define the targets for each step. This gives further confidence in the process.

The difficulty of making quantitative comparisons across different host rock formations (e. g. salt, clay and granite host rock) was discussed. Firstly, there is a need to adapt the geoscientific investigation programme to the respective host rock. As shown for the Canadian approach, different investigation methods have to be used for granite rocks and sedimentary rocks. Secondly, the comparison of sites in different host rocks is hindered by the facts that to some extent different processes have to be considered, those processes might act in different ways and the safety concepts are different for different host rocks. For direct numerical comparison, additional problems arise e. g. from the fact that for a repository in rock salt no radionuclide release may occur under the normal evolution scenario, whereas in other formations this is usually not the case.

An approach developed in Germany which is a combination of a (i) so-called Verbal-Argumentative-Method (VAM) based on a comparison of the safety function “robustness” of the repository system in a verbal-argumentative stepwise approach and (ii) Probabilistic-Calculations-based-Method (PCM) based directly on quantitative analyses and model calculations. For application of both methods sufficient geoscientific knowledge of the sites is needed.

3.2.1.5 Geological versus societal criteria

Part of the discussion was directed to the role of socioeconomic aspects in the siting process. Firstly, it was stated that there is a need to fulfil both geoscientific and societal criteria for a successful siting process. The judgement of the quality of a site with respect to safety is strongly based on geoscientific criteria but societal criteria frame the process.

There is a danger in trying to select the ‘best site’ from a geoscientific point of view even in the ranking of sites. Firstly, it might be hard to define the ‘best site’ and to find it, particularly if different host rocks are considered. Secondly, it might turn out that the ‘best site’ is not socially acceptable and this will then cause problems in gaining confidence in another site, which is seen as only ‘second best’. It was proposed, instead, to talk in terms of an ‘optimal site’, since optimisation includes other factors, including societal factors. However, there is a general tendency to avoid ranking sites. Instead, it is proposed not to differentiate between sites, distinguishing only between those sites that can provide the required safety and those that cannot.

In an optimisation process economics should not be overlooked. If the quality of a site is limited, engineering measures might still be applied to achieve an acceptable safety case. However, the costs of implementation may be very high in such a case. There should be a preference for a site that has the natural ability to contain radionuclides with respect to safety, but it is, of course, the whole system performance what matters.

One observation from the Swiss case is that geoscientific criteria play a key role in the siting process and this fact is strongly supported by the public increasing their confidence in the process. In addition, consultations aimed at gaining stakeholder support for the whole process including the role of the involved organisations and for establishing siting criteria are very important, as shown from experiences in the UK and Switzerland (Swiss Sectoral Plan). Generally, the whole siting project should favour a community's well-being. In the Canadian process a strong interaction between the public stakeholders and the implementer has been established including joint field visits with a detailed explanation and discussion of the next steps to the public as well as participation of implementer staff in ritual ceremonies of the aborigines, to demonstrate respect of local community values.

In general, advanced programmes show that a systematic, stepwise process with open communication of progress and discussion of remaining safety issues is one factor of success. This includes empowerment of local people and might go as far to provide the right of veto up to certain stages. However, the latter is not valid for every country. Also support to local communities in matters of expertise and some joint development/outreach/support programme is part of the fair play with the local community.

A good balance between siting studies and concept development can help clarify safety functions. Requirements can be developed from the safety functions. In particular at early stages, assessments of safety must not necessarily involve dose calculations, but rather the evaluation of barriers using other indicators. This, however, would not lead to a full safety case, but basically every stage of the process involves assessing safety in some way (see discussion above). It was mentioned that the NEA status report "indicators in the safety case" can be of help, as it discusses several examples of barrier-related indicators to be used with respect to the safety functions /NEA 12/.

3.2.2 Criticality and safeguards

The IGSC topical session in 2017 was devoted to the assessment of criticality and safeguards in a deep geological radioactive waste repository. The topical session dealt with experiences from assessments of criticality safety and application of safeguards in the different member countries of the IGSC. For criticality the objectives were to:

- explore how members are planning to manage or have demonstrated criticality safety in the post-closure phase of a repository;
- identify dependencies on host rock formation, repository design, waste package materials, etc.;

- compile and evaluate measures to guarantee long-term criticality safety;
- evaluate regulatory views on how to demonstrate criticality safety for the repository.

For Safeguards the objectives were to:

- compile and evaluate strategies to provide safeguards for the nuclear material in the repository with or without retrievability requirements (according to national legislation);
- evaluate regulatory views on how to demonstrate safeguards for the repository.

The following presentations were given:

- Criticality effects of long term changes in material composition and geometry in a damaged disposal canister. *Kastriot Spahiu, Lennart Agrenius, SKB, Sweden*
- Long-term criticality safety: challenges and research, German perspective. *Robert Kilger, GRS, Germany*
- Study on criticality in deep geological disposal in Japan*. Hitoshi Makino, JAEA, Japan*
- Demonstrating post-closure criticality safety of the UK geological disposal facility. *Robert Winsley, RWM, UK*
- Post-closure nuclear criticality safety assessment for the French Cigéo clay repository. *Clement Lopez, Andra, France*
- Post-closure Criticality Review and Safeguards Considerations for a Proposed High-level Radioactive Waste Repository. *Jack Gwo, US NRC*
- Status of Criticality and Safeguards Management in Canada. *Helen Leon, Neale Hunt NWMO, Canada*
- Posiva's approach to criticality management and safeguards. Anssu Ranta Aho (TVO), *Barbara Pastina, Marie Lahti Posiva, Finland*
- Safeguarding geological repositories in the context of national legislation – the German case. *Irmgard Niemeyer, FZJ, Germany*
- Application of Safeguards to Geological Repositories. *Marius Davainis, IAEA*

The main results from presentations and discussion are summarized in the following.

3.2.2.1 Regulatory aspects on criticality

The regulatory requirements given for the assessment of long-term criticality safety differ widely for each country. In some countries only very general requirements are given, e. g. in Germany, where it is stated that „… the exclusion of self-sustaining chain reactions for both probable and less probable developments must be proven”. There is no specific requirement how this has to be shown or any specific target value given for the effective neutron multiplication factor, k_{eff}, which must not be exceeded. In Japan, where the waste policy was based on reprocessing and vitrification of spent fuel, more back-end flexibility was recommended after the Fukushima accident. As a consequence, direct disposal is now under the R&D stage, but there are no specific regulatory requirements with respect to direct disposal including criticality yet.

In other countries the requirements are formulated in a very specific way. In Sweden the effective neutron multiplication factor, k_{eff}, including uncertainties should be < 0.95 in the repository and <0.98 in unlikely events or accidents. In Finland such requirements are so far only given for repository operation. STUK YVL Guide B.4 states that the effective multiplication factor k_{eff} will not exceed the value 0.95 under normal conditions or in anticipated operational occurrences and the value 0.98 in other design basis scenarios. Another requirement from the Finish YVL guide D.5 states that “… the spent nuclear fuel contained in a disposal canister shall remain subcritical also in the long term. The design shall accommodate conditions where the leak-tightness of the container has been lost and the container has sustained mechanical or corrosion-induced deformations”. This implies very specific requirements on the container construction with respect to criticality safety.

The environment agencies’ Guidance on Requirements for Authorisation (GRA) for a geological disposal facility in the UK requires a demonstration that “the possibility of a local accumulation of fissile material such as to produce a neutron chain reaction is not a significant concern” and it further states that “the environmental safety case should also investigate, as a ‘what-if’ scenario, the impact of a postulated criticality event on the performance of the disposal system)“.

3.2.2.2 Scenarios for criticality safety assessment

For the demonstration of long-term safety as well as of criticality safety it is needed to make plausible assumptions of the future evolution of the repository, i. e. to define scenarios. For long-term safety assessment usually a transparent and traceable approach is applied to derive probable and less probable scenarios to be considered in the calculation cases.

For demonstration of post-closure criticality safety such a systematic and transparent approach is not available so far and quite different approaches with respect to scenarios are applied. The evaluation of the presentations indicates that the stage of the repository programme as well as regulatory requirements influence the scenario selection. In Germany, where the repository programme is still in a pre-siting stage, for the recent VSG (Vorläufige Sicherheitsanalyse Gorleben) study partly very conservative assumptions with respect to the evolution of the repository system as for example an early flooding of the waste containers is taken as a basis. This process has not been identified as being part of a probable or less probable scenario and was not considered in the calculations for long-term safety assessment.

On the other hand, for demonstration criticality safety in the Swedish safety case, where the Forsmark site is already selected and the repository process is approaching the construction phase, the same scenarios, namely (i) canister failure due to corrosion (for advective conditions caused by bentonite erosion) and (ii) canister failure due to shear load caused by a large earthquake, have been considered in criticality safety and long-term safety assessment. Nevertheless, the assumption that one container is filled with water after a 100 y is also very conservative.

Transparency and credibility might be increased, when scenarios applied for both, long-term and criticality safety, are more consistent. A step towards a more systematic approach of scenario derivation for consideration of criticality events might also be the use of features, events and processes (FEP). FEP catalogues are widely used in scenario derivation for long-term safety assessment to increase transparency and reach comprehensiveness. Such A FEP based approach was introduced by the US presentation, where 16 FEP on criticality were identified and documented.

However, as already discussed above, in some countries the selection of specific scenarios for demonstration of criticality safety is required by legislation. The UK guidance demands the investigation of the consequences of a what-if scenario assuming a postulated criticality event in the repository. The analysis of such a criticality event in the repository was also analysed in the French, Swedish and Japanese study. Typical results from the UK study showed that consequences from quasi-steady-state transient criticality events of one container occur localised, the power is below 2kW and a temperature rise in the host formation of above 10 °C is limited to an area of just a few meters.

Similarities in the approaches are observed with respect to the following. Nearly all studies consider the potential of criticality within and outside of the canisters. Inside the flooded canister it is usually distinguished between an intact waste form on the one hand and the formation of corrosion products and degraded/fragmented fuel on the other hand. For the latter case in some studies a homogeneous mixture of fuel, corroded metal and water was assumed and in other studies more thoughts were given to the formation and distribution of the corrosion products. However, as shown in the Swedish study, there is a lack of data especially for distribution and hydration of corrosion products formed after very large time spans. For these not even archaeological data exist. In such cases expert judgement was used to define the considered systems. Outside the container possible accumulation processes for the fissile isotopes are identified and the potential for the system to become critical is estimated for them.

3.2.2.3 Methodological approach to criticality assessment

Generally, it seems that standardized approaches for criticality assessment for DGR are not available, but methods have been adapted from nuclear industry applications.

Deterministic calculations are always performed and necessary in any case. However, for consideration of parameter uncertainties several organisations perform also probabilistic calculations, complementing and supporting the deterministic calculation cases. Another wide fold strategy to consider uncertainties is the use of conservative assumptions. Nearly all studies assume a more or less early flooding of the container. Since the fissile isotope ^{239}Pu decays to the fissile isotope ^{235}U in many cases the most critical point in time, where the highest effective neutron multiplication factor occurs, is addressed. Another example for very conservative assumptions was given in the Canadian study. In the considered scenario a fast dissolution of spent fuel, which is only possible under oxidizing conditions, is assumed. Dissolved uranium is then efficiently accumulated by immobilization; such a process is only expected under reducing conditions. This scenario causes highest consequences and even in this case it was shown that no criticality occurred. But, such a scenario is inconsistent and not realistic; hence it was recommended to address more realistic and consistent scenarios, unless otherwise required by regulations.

3.2.2.4 Host-rock, design and material specific aspects on criticality

One interesting observation is related to large differences in criticality safety demonstration caused by specific characteristics of the host-rock, the design or the waste material itself. With respect to the host rock the occurrence of highly mineralized water is a clear advantage with respect to criticality safety. This is particularly due to the neutron absorbing properties and the high natural abundance of 75.76 % of the isotope ^{35}Cl. Due to its relatively high thermal absorption cross section of 43.7 barn it acts as a neutron absorber significantly decreasing the reactivity and therewith the probability of criticality. This is illustrated by reduction of the effective neutron multiplication factor, k_{eff} in saturated brines especially in salt rock compared to systems with pure water, as for example investigated in the German study.

For the container design, typically the main criteria originate from operational requirements and not from criticality considerations. However, there are also design issues, which are of relevance for criticality safety and in order to avoid a high potential for criticality, (preliminary) criticality assessments at an early stage of container conceptualization are recommended. The number of fuel assemblies and thus amount of fissile material per container is of course important and some basic investigations for representative spent fuel containers have been performed for example in Japan. In this context it is of relevance, how much burn-up credit need to be taken into account for reaching criticality safety. Usually burn-up credit is allowed to be included but it is not mandatory. And it need also to be considered that some engineering materials like concrete or bentonite can act as reflectors and therewith negatively impact the occurrence probability of criticality.

Another issue on container design is related to the consideration of the direct disposal of the storage and transport container for spent fuel elements Castor, which is currently under discussion as one disposal option in Germany. To reduce the potential for criticality in the repository it is proposed to use magnetite infill in the void volumes of the Castor container.

Finally, it is the waste itself, whose properties impact the potential for criticality. For example, the majority of the Canadian fuel wastes from nuclear power plants are CANDU bundles. CANDU fuel is not enriched and contains the natural fraction of U-235 of 0.72 wt._%, i. e. much less fissile material compared to spent fuel. Such CANDU fuel cannot go critical under any realistic scenarios, neither in the used fuel packing plant, nor in the deep geological repository. The same is true for vitrified waste from reprocessing, which represents by far the majority of the high-level radioactive waste in France. The result of the French criticality safety assessment for this type of waste, where uranium and plutonium is partitioned from the waste, showed that the likelihood of a criticality in the repository is indeed impossible.

3.2.2.5 Safeguards aspects

Safeguards for fission material are mandatory for deep geological repositories. Already in 1988 experts recommended that IAEA should not terminate safeguards on spent fuel before or after emplacement in a geological repository.

Particularly during the last technologies have been compiled and described which are potentially useful for safeguarding geological repositories. Within the project ASTOR (Application of Safeguards to Geological Repositories) proposed technics and methods have been compiled /IAEA 17/ as

- design information verification,
- non-destructive assay verification,
- containment & surveillance,
- satellite imagery & geophysical techniques, and
- long-term data management.

In order to implement the IAEA safeguards continuous dialogue between all stakeholders – the state, operators and IAEA is desirable. An example is the EPGR project in Finland and Sweden, where safeguard approaches for encapsulation plants and geological repositories are developed and the appropriate equipment and technologies are tested integrated and installed in cooperation with IAEA.

General challenges are the exceptionally long life-cycle of the projects, the application of “best available” techniques for spent fuel measurements and maintaining continuity of knowledge while transporting disposal canisters. Further challenges for deep geological repositories are that

- nuclear material will not be accessible for direct verification,

- disposal canisters will become inaccessible after a tunnel is backfilled or the repository is closed,
- the design of the facility will not be frozen – excavation of new tunnels will be taking place at the same time as other tunnels are being backfilled,
- only a small part of the facility will be visible above ground,
- undeclared areas can be ‘hidden’ behind declared tunnels, and
- access routes to the repository may be excavated before or during its operation life.

The status of implementation of safeguards concepts and measures widely differs. In regulations of some countries safeguards are not specifically addressed (e. g. Canada) whereas in other countries they are explicitly mentioned as in different Codes of Federal Regulations (CFR) in the USA. In the guide on nuclear safety in Finland specific requirements related to the disposal of spent nuclear fuel are contained. Several specific requirements about accountancy and control systems during the operational phase were described. A strategy for providing safeguards after repository closure, including responsibilities, information about the repository, and documentation was given. Retrievability is included as a condition in the construction license. It considers the identification of disposal canisters and the control of backward flow of nuclear material.

3.3 EGOS

The expert group on operational safety (EGOS) was established by IGSC in 2012 and hold its kick-off meeting in June 2013. The mandate of the group was extended to the end of 2019 by IGSC in 2017. The work program at the beginning was

- fire assessment in deep geological repositories,
- ventilation in underground facilities,
- an NEA “hazard” database,
- operational hazards,
- waste acceptance criteria, and

- assistance of the WAC task group of EGOS to discuss criteria required to address operational safety aspects (e. g. radiological protection and limits, waste packaging design and specifications, etc).

In the years 2014 to 2017 annual meetings with all EGOS members took place; additionally, selected members met in working groups on special topics, e. g. on fire risk, ventilation, or hazard database. In the actual work program of the years 2018/2019 three topics have been added:

- demonstration of safety and reliability of transport and emplacement systems,
- methodologies and approaches of safety assessment for the operational period, and
- discussion of the relationship between operational safety and long-term safety, and how they should be addressed.

The main outcome of the discussions up to now in summary is:

Fire risk & Ventilation: A draft version of the summary report exists and will be supplemented by a chapter about challenges in installing a ventilation system. The report contains an overview of current disposal concepts as well as fire risk management and ventilation approaches. Fire scenarios are formulated, and potential future work is proposed in an attempt to induce more in-depth evaluations and investigations.

Hazard database: Initially an electronic version of a database of operational hazards was in discussion. This idea was replaced by a text file and spreadsheet solution based on a hazard list in UK. A draft version of the list exists and is intended to be completed by members in 2018. Results will be compiled in a final report. The list will be based on information of operational hazards from mines (uranium and non-nuclear) and nuclear facilities. Waste handling and transport activities, including transport vehicles and access shaft transport, as well as concurrent construction and waste emplacement activities are taken into account. A method for assessing and anchoring the identified hazards in the safety case will be developed.

Demonstration of safety and reliability of transport and emplacement systems: This task group hold one meeting in 2016. It identified the relevance of repository concepts and waste packages for the design of transport and emplacement systems. According to the DGR program evolution further 1:1 scale demonstrators are proposed. A project report is in development.

Waste acceptance criteria: Using a questionnaire, participants compiled waste acceptance criteria of the member states. It turned out, that preliminary criteria exist in most national programmes, but many countries have used other terminologies to denote such criteria (mostly due to their early developmental stage of their repository programmes). For the same reason, some members indicated this topic is not their priority at present (e. g. Switzerland, Germany). Existing WAC seem to focus mainly on operational safety. There are not so many criteria derived from long-term safety aspects. Further requests to other organisations regarding WAC are ongoing and a further meeting is envisaged.

The annual meetings of EGOS served as an exchange forum of national experience in the fields mentioned above. Not all of the information resulted in reports up to now. The information exchange was necessary to create a common base for detailed work and to select relevant topics for further discussions which result in final reports.

A joint workshop of NEA (EGOS) and IAEA (GEOSAF project) was performed in July 2016 in Paris. In the first part of the workshop, results of the two projects and details from national programmes were presented. General aspects of operational safety, risk management, installation of ventilation systems, transport and emplacement techniques, and repository designs have been on the focus as well as lessons learnt from the WIPP site hazard. In the second part the regulatory framework in different countries has been discussed. The project MoDeRn was presented and requirements for monitoring and transport management were discussed. In the third part the focus was on the interactions between operational safety and long-term safety. Some preliminary results from national programmes were discussed and it was concluded that further treatment of this topic is essential for the safety case.

The topic on methodologies and approaches of safety assessment for the operational period has not yet started. It is planned to compile information on operational safety assessments and the interaction between operational and long-term safety aspects. This topic came up in a discussion about the consequences of a fire event in a mine and remediation activities. The consequences of such an event on long-term safety have not been addressed yet.

3.4 Salt Club

The “Expert Group on Repositories in Rock Salt Formations (Salt Club)” was established in 2012 by OECD/NEA under the auspices of the IGSC by representatives from organizations in the United States, Germany, Netherlands and Poland involved in the safe disposal of radioactive waste in rock salt. Beginning 2018 United Kingdom and Romania joined the Salt Club.

The Salt Club has the general objective of effectively developing and exchanging scientific information and shared approaches as well as methods to develop and document an understanding on rock salt as a host rock formation for a geological repository. Mission and objectives are written down in the Terms of Reference (http://www.oecd-nea.org/rwm/saltclub/). In general, scientific issues are addressed within the Salt Club that refer to the long-term behaviour of the repository system and its isolation functions. Also, diverse methodological aspects regarding safety cases and performance assessments are dealt with, e. g. models, reliability and quality of data. Natural analogues are explicitly addressed within the geochemical and the Safety Case topics.

The Salt Club holds regular annual meetings at which its work programme and individual projects are established, updated and reported about. Typically, about 30 to 40 individuals participate at the annual meetings. The Salt Club mandate spans two-year periods, respectively, and is then renewed by IGSC. Since its creation, the Salt Club has published several scientific reports addressing specific topics and it has contributed to the organization of several workshops as follows:

- the potential of natural analogues for contributing to safety cases for repositories in salt formations (a report was published in 2013 /NEA 14a/);
- the scientific basis for granular salt reconsolidation, since this process has direct implications with respect to engineering, design, construction, evolution and performance of lateral closure systems in a salt repository (a report was published in 2014 /NEA 14c/);
- the evaluation of the potential role of microorganisms in salt-based radioactive waste repositories using available information on the microbial ecology in hypersaline environments (a report was published in 2018 /NEA 18d/);
- a series of workshops on actinide brine chemistry (ABC Salt III in 2013, ABC Salt IV in 2015, ABC Salt V in 2017).

The potential for microbiological effects to impact the long-term performance of a salt-based radioactive waste repository was assessed in /NEA 18d/ based on the current understanding of microbial processes and microbial communities in high ionic strength systems. Microbial communities can be found in hypersaline settings. They are, however, limited in both structural and functional diversity when compared to other environmental matrices, such as soil. The reason for this limitation is that in order to survive at high-salt concentrations, such organisms must osmotically balance their internal and external environments, limiting their ability to perform certain modes of metabolism based on the energy required for survival and the energy derived from a given metabolic reaction. Because the biogeochemistry of other deep geological settings differs significantly from that of subterranean salt, it is not always possible to extrapolate microbial activity from one type of site to another. The lack of data and the resulting uncertainty surrounding microbial processes in high ionic strength repository settings has meant that performance assessments and safety cases had been conservative in their predictions of potential microbial impact.

Although some potential impacts have been identified, one key conclusion of the report /NEA 18d/ is that the expected environment in a salt repository is unlikely to be conducive to the level of microbial activity needed to incur a significant impact on repository performance. This view contrasts with what has often been observed in near-surface or low ionic strength environments where higher activity and diversity have been predicted. Thus, the usual assumptions about microbial processes do not always apply to salt-based geological settings. Salt-based repositories may have additional microbial considerations, such as those shown in Fig. 3.2.

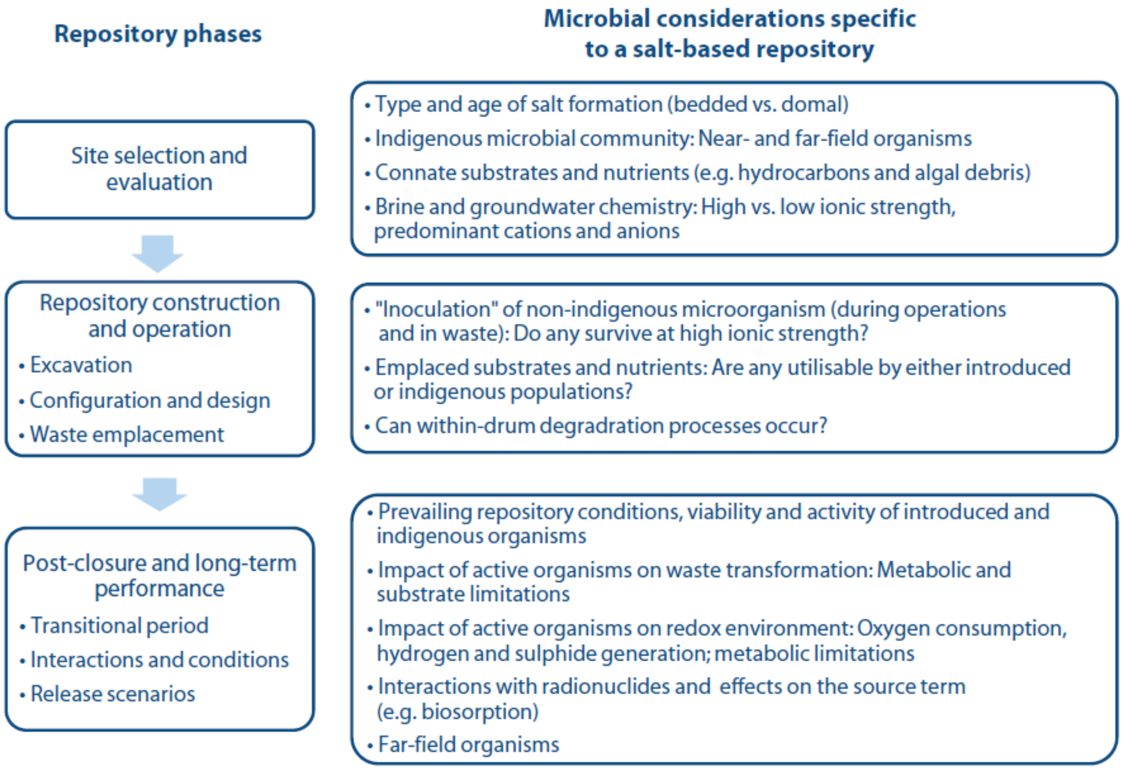


Fig. 3.2 Repository phases and microbial issues to be considered for salt-based repositories /NEA 18d/

The main questions for a salt-based repository concept are: will anything survive and, if it does, will it do anything? The negative results obtained when trying to grow salt-indigenous organisms under repository conditions should be viewed as meaningful. These negative findings can be supported by community characterisation studies and genome sequencing so as to determine the feasibility of microbial activity under given conditions. Areas in which data can be generated include any microbe-radionuclide interaction studies. Due diligence in all these areas can help mitigate the remaining uncertainty surrounding the effects of microorganisms on salt-based radioactive waste repositories.

3.5 Clay Club

The Working group on the Characterization, the Understanding and the Performance of Argillaceous Rocks as Repository Host Formations ("the Clay Club") was established in 1990 with the aim to promote the discussion of scientific research in argillaceous formations. Its role is to examine those argillaceous rocks that are being considered for the deep disposal of radioactive waste, which range from soft clays to indurated shales.

During the last years three topics were in the focus of the Clay Club work:

- investigation of clay characteristics on the nano scale,
- update of the Clay Club catalogue (CCC), and
- investigation of the binding state and mobility of water in clay-rich sedimentary rocks (CLAYWAT project).

Clay rocks are composed of fine-grained minerals with pore sizes in a range from < 2 nm up to > 50 nm. The water flow, solute transport and mechanical properties are largely determined by this microstructure, the spatial arrangement of the minerals and the chemical pore water composition. This concerns for example the anion accessible porosity and macroscopic membrane effects like chemical osmosis and hyperfiltration as well as geomechanical properties and the characteristics of two-phase flow properties, which are relevant for gas transport. In order to deeper investigate this topic, two workshops have been performed during the last years. A first workshop on "clay characterisation from nanoscopic to microscopic resolution" was held in 2011 /NEA 13c/. Key topics were the current state-of-the-art of different spectro-microscopic methods, new developments addressing the knowledge gaps especially on the microscale in clays and results from molecular modelling in comparison to experiments. A second workshop connected to the EUROCLAY 2015 was devoted to the topics (i) pore structure and connectivity, (ii) chemical information under high spatial resolution, (iii) gas/water and ion mobility in tight formations, (iv) upscaling and implementation in model approaches and (v) rock mechanics. Details of the outcome are documented in /SCH 16/. Besides others the workshop demonstrated the advanced application of experimental techniques such as neutron diffraction and scattering, µ-XAFS, nano-SIMS, TEM, AFM, nano-XCT, BIB-SEM, and NMR, to yield new and fundamental insights into physical/chemical processes acting on the solid phase on a microscopic scale, i. e. down to the molecular scale /SCH 16/. However, the lack of standardized procedures for specific approaches to sample preparation and preservation was mentioned. The important role of molecular-modelling techniques was emphasized, which allows elucidation, at an atomic scale, of the mechanisms of radionuclide sorption onto clay minerals, of interfacial water structuring, and of the migration behaviour of solutes (anion, cation) through compacted clays.

One of the first initiatives of the Clay Club was to gather the key geoscientific characteristics of the various argillaceous formations that are – or have been – studied in NEA member countries in the context of radioactive waste disposal. The results were documented in the Clay Club Catalogue of Characteristics of Argillaceous Rocks (CCC, /NEA 05/). This report is currently being revised by providing new datasets for a selected number of argillaceous formations, and by providing an expanded discussion of (i) the formations and their properties, (ii) the nuclear waste management organizations responsible for implementation of the deep geological repository concept, (iii) the design concept proposed for a DGR in the respective countries and rock formations, and (iv) some of the favourable properties of these formations. A key goal of this report is to present the data in a manner that allows reasonable comparability (in both scale and methods) of the included parameters, as a means to demonstrate the overwhelming capacity of clay-rich formations to securely contain and isolate nuclear waste from the natural environment.

In 2016 the Clay Club started the CLAYWAT Project, which is primarily aimed at examining the state of the art in understanding of the binding state and mobility of porewater within a broad range of indurated argillaceous sediments considered for long-term radioactive waste management purposes. The project consists of three stages: In the first stage a literature study is performed to evaluate laboratory techniques which can provide information on the binding state of pore waters. This literature review will be used, in part, to identify and select methods for application during the second stage of the study in a comparative study using preserved clay rich samples from CC member countries. The third and final stage of the work program will involve the interpretation and synthesis of the laboratory data. The project is nearing completion of stage 1 and selected experimental methodologies and responsible laboratories have been compiled. Nuclear Magnetic Resonance (NMR) is considered as one of the most powerful methods to examine the binding state and mobility of water in clay-rich sedimentary rocks. Other methods, which might be used are e. g. pore size distribution by nitrogen and water absorption isotherms, thermogravimetry, and neutron diffraction and scattering measurements.

3.6 Crystalline Club

The Crystalline Club (CRC) of the OECD/NEA was established in December 2016 and is currently in the phase of the first mandate (December 2016 – December 2018). Current member countries are: Czech Republic, Canada, Germany, Japan, Romania, Russian Federation, Spain, Switzerland and USA. The focus of the current CRC activities is on the compilation of a report on the status of radioactive waste disposal in crystalline formations in CRC member countries. The contents of the report will give an overview on international collaboration and research activities and the current concept and state of art of deep geological repository (DGR) development in the CRC countries. Completed and ongoing research will be summarized addressing the following topics:

- characterization of the geosphere (site characteristics, laboratory research, grouting technology and excavation damaged zone (EDZ)),
- safety functions of the geosphere and performance requirements of the engineered barrier system (thermal, hydraulic, mechanical, and chemical (THMC); seal design, buffer/backfill/seal emplacement, voids filling in a DGR in crystalline rock), and
- safety assessments (assessment context and system description, FEP and scenario analyses related to crystalline rock, modelling, uncertainties/confidence in assessment results).

It is aimed at completing the report by the end of 2018. The report will be reviewed by external reviewers before publication.

Topics of interest for future work of the Crystalline Club and the potential focus of the CRC during the following years were compiled and discussed. The following topics are of interest for the member countries.

- International regulations in the field of deep geological repositories:
  All countries, that have ratified the IAEA "Joint Convention on the Safety of Spent Fuel Management and on the Safety of Radioactive Waste Management", have to bring their regulatory framework in line with international requirements. Construction and operation of a DGR is a long process. During this time, the legislation might be changed, potentially causing difficulties in adapting the licensing process and in planning corrective actions to comply with requirements. That is why it is important to be well informed about international developments and planned significant changes in the recommendations of international organizations.
- Comparison of national criteria and radioactive waste disposal plans:
  For defining potential topics of future collaboration in the CRC, it is important to get an overview on the different national stages of the siting process in a first step. This topic is approached by a comparison of safety criteria, methodology of its applica-

tion in the current stage of siting process and how the criteria are changing from site screening during investigation to licensing. The main question is how to adapt and focus criteria from the general concept to a site and design specific stage.

- Research in the process of the disposal construction:
  Research programs for the investigation of a potential repository site include the above surface and the subsurface investigation. Subsurface investigation programs are planned beforehand and need to be adapted during the construction of the repository, as new data are becoming available, e. g. on the stress-strain state of the site. Therefore, a review and compilation of research programs, research methods and equipment used would help to provide a strategy for the planning and adaptation of investigations programs before and during the construction phase of the repository.

- Mutual influence of engineering barriers from cement and clay and host rock during disposal of radioactive waste:
  Research on the long-term forecast of the mutual influence of the barriers revealed that the degradation of the barriers is not only fostered under elevated temperature and pressure conditions, but also under normal conditions. Several older publications indicate a negative mutual influence of bentonite and cement as materials of engineering barriers. Focusing on this topic in future Crystalline Club activities would help to bring all members up to date with the current research in this field, and to identify the effect of cement and clay on crystalline rock, e. g. when filling fractures.

- Determination and handling of discontinuities and fracture networks in crystalline rock for the safety case:
  In crystalline rocks, different orders of discontinuities are existent, from macro to micro scale. For the safety case of a deep geological repository, it is essential to know the different discontinuity types and their relevance for the thermal, hydraulic, mechanical and chemical properties of the rock. Important questions concern the field and laboratory methods for discontinuity characterization and their handling in numerical models. Evaluating the impact of the discontinuity properties on the long-term safety is an important step towards the safety case.

Some of these topics were addressed by the first topical session of the CRC during the second plenary meeting in Mizunami, Japan in June 2018. The title of the topical session was “Process Comprehension using Under Ground Research Laboratory” and aimed at presenting (i) a project overview on the Mizunami Underground Research Laboratory (MIU) and (ii) research and development (R&D) results. Special focus was on discontinuities and their relevance for THMC; methodology for discontinuity characterization and modelling; long-term forecast of mutual influence from engineering barriers; and identification of common challenges in this area among CRC countries. Speakers were from JAEA and NUMO (Japan), SNL (USA) and SÚRAO (Czech Republic).

During the plenary meeting in Japan, the future program of work (PoW) was discussed. A proposal from the Czech Republic concerns a compilation of rock properties relevant to safety functions. In a first step, the process from data aquisition in the field, their incorporation into geosphere and safety models and their interpretation will be described. The goal is to define all necessary parameters that are needed to transfer geological and hydrogeological models to safety assessment models, including a description of modelling approaches (geosphere simplification). Eventually, guidelines for siting criteria development can be derived. The proposed working plan includes three workshops on: (i) data acquisition, preparation for modelling, accuracy, precision, data management, (ii) modelling: description of workflow, computational approach, exchange formats, input and output and (iii) the development of siting and safety criteria. Other suggestions are still welcome. Proposals The program of work will be discussed and decided on in the course of a CRC bureau meeting to be held in September 2018.

3.7 NEA State of the art report to assess modelling and experimental approaches

In the frame of the TDB project the OECD/NEA initiated state of the art report on the topic high ionic strength solutions – state of the art report to assess modelling and experimental approaches" /NEA 19/. The report illustrates to which extent geochemical processes in high mineralised solutions can be modelled by the Pitzer approach. The German contribution to this report was supported by this project and comprised the analysis of the status for heavy metals, particularly iron and lead. Selected results are presented in the following.

While for the systems $FeCl_2$ - Na, K, Mg, Ca - H_2O at 298.15 K available data seem sufficient to derive a Pitzer model (see Fig. 3.3 and Fig. 3.4), the situation for the same systems with $FeSO_4$ is dissatisfactory.

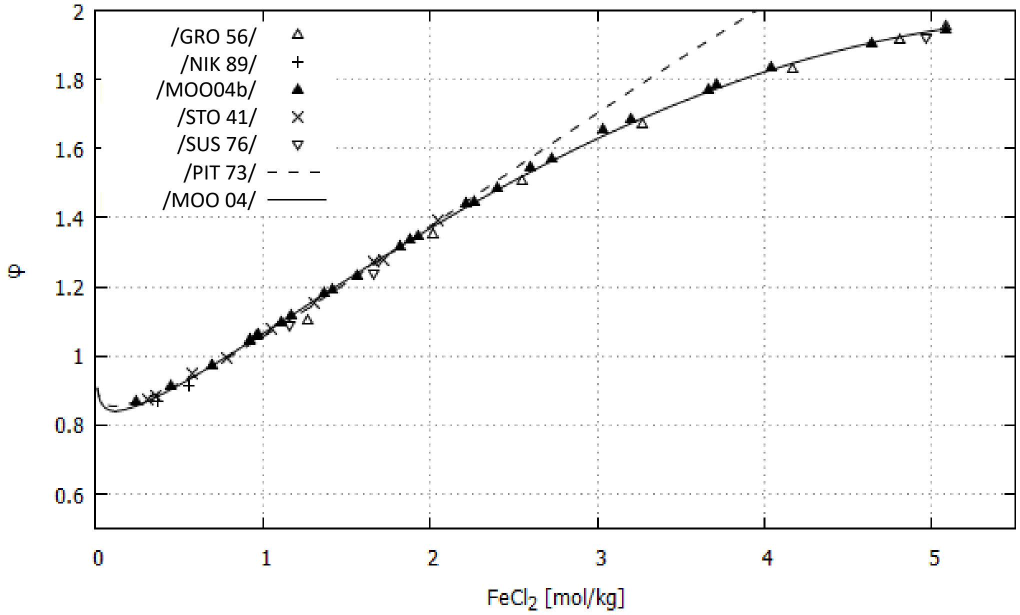


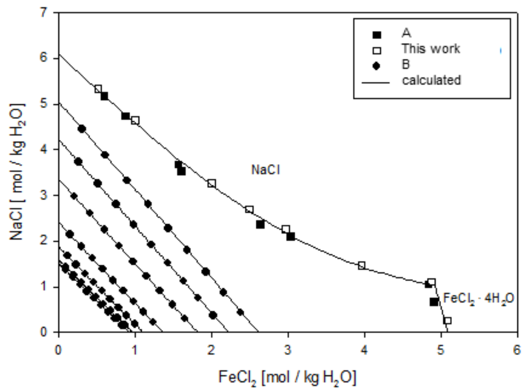
Fig. 3.3 Osmotic coefficients for the system Fe(II) – Cl – H_2O at 298.15 K

For the undersaturated binary system $FeSO_4$-H_2O essentially one source of data is available only. For ternary coefficients solubility data are available. However, they could exert an undesirable bias on ternary Pitzer coefficients used for other systems which are of real importance for nuclear waste disposal.

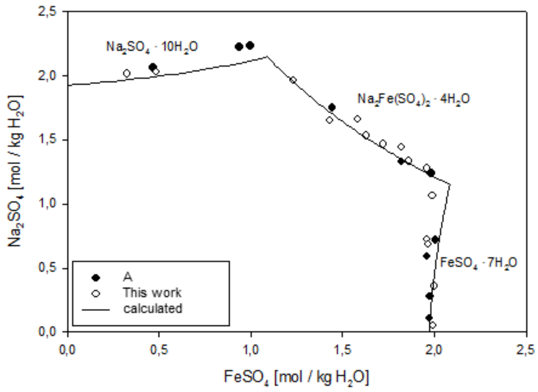
For temperatures above 298.15 K vapour pressure data are available for $FeCl_2$-H_2O only, and only from a single source, see Fig. 3.5. Available solubility data might be useful for deriving Pitzer models applicable for industrial purposes but to a much lesser extent for the sake of nuclear waste disposal.

While for chloride systems isopiestic measurements could be employed to close data gaps, sulphate systems seem to defy this method due to sluggish equilibration. Considering useful measures to enhance the situation towards a Pitzer database for nuclear waste disposal, it is recommended to conduct further isopiestic measurements where this seems feasible (chloride systems), and to complement them with solubility studies for solid phases relevant for nuclear waste disposal. In the latter case, sulphate concentration could be a boundary condition varied to derive respective Pitzer coefficients.

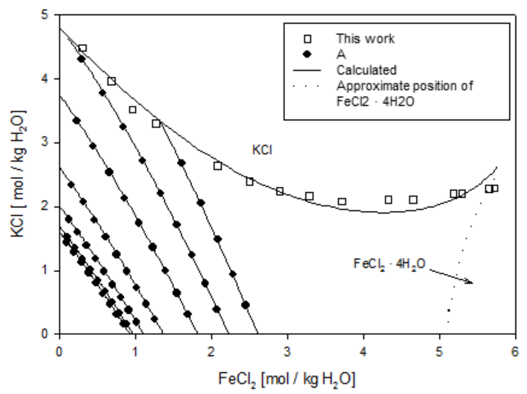
As to ferric iron, many studies were motivated by either the interest in understanding industrial process solutions, or the formation of ferric precipitates under (hypothetical) conditions on Mars, or the quantification of ferric hydrolysis in seawater. With regard to conditions relevant for nuclear waste disposal neither the low-pH studies for industrial processes nor the low-temperature data assessments conducted for applications in martian surface geochemistry seem to be of much relevance.



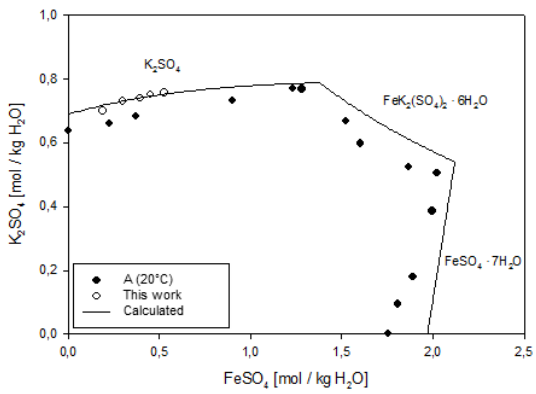
[A] = Afonickin, O. V.; Gajdukova, T. I. (1975): Rastvorimost´ solej v sistemach NaCl- FeCl2-H2O i MgCl2-FeCl2-H2O, Trudy Vsesoyuz.Nauch.-Issledovatel Inst. Galurgii, Ministersvo Khim. (74), 30-34.
[B] = Moog, H. C.; Hagemann, S.; Rumyantsev, A. (2004): Isopiestic Investigation of the Systems FeCl2 - (Na, K, Mg, Ca) - Cl - H2O at 298.15 K, Z. Physikal. Chemie 218, 1063-1087.



[A] = Zdanovskij, A. B.; Sokolov, I. D.; Kydaseva, A. N.; Ceremnych, P. M.; Safrygin, A. N. (1974): Rastvorimost´v trexkomponentnych vodno-solevych sistemach c sulfatom zeleza (II), Trudy Vses. Naucno-issled. Proektn. Inst. Galurgii (72), 90- 101.



[A] = Moog, H. C.; Hagemann, S.; Rumyantsev, A. (2004): Isopiestic Investigation of the Systems FeCl2 - (Na, K, Mg, Ca) - Cl - H2O at 298.15 K, Z. Physikal. Chemie 218, 1063-1087.



[A] = Legrand, M.; Paris, R. A. (1966): Étude à 20°C des systemes: eau, sulfate ferreux, sulfate de potassium; eau, chlorure ferreux, sulfate ferreux; eau, chlorure ferreux, chlorure de potassium; eau, chlorure de potassium, sulfate de potassium, Bull. Soc. Chim. Fr. (8), 2699-2701.

Fig. 3.4 Isoactivity lines and solubilities in the systems $FeCl_2$ – NaCl – H_2O, $FeCl_2$ – KCl – H_2O, $FeSO_4$ – Na_2SO_4 – H_2O, and $FeSO_4$ – K_2SO_4 – H_2O at 298.15 K (from /MOO 04b/)

Unlike the situation with ferrous iron, speciation of ferric iron, especially with hydroxide, cannot be neglected if aqueous systems are regarded with relevance for nuclear waste disposal. Due to the extent of complex formation the task of building up a database for ferric iron, internally consistent with respect to stability constants, solubility constants, and Pitzer coefficients, might evolve in an unsurmountable task. For sure a database which extends to strongly acidic and may be strongly oxidizing conditions would be useful for other industrial applications, but at the same time irrelevant for the sake of nuclear waste disposal.

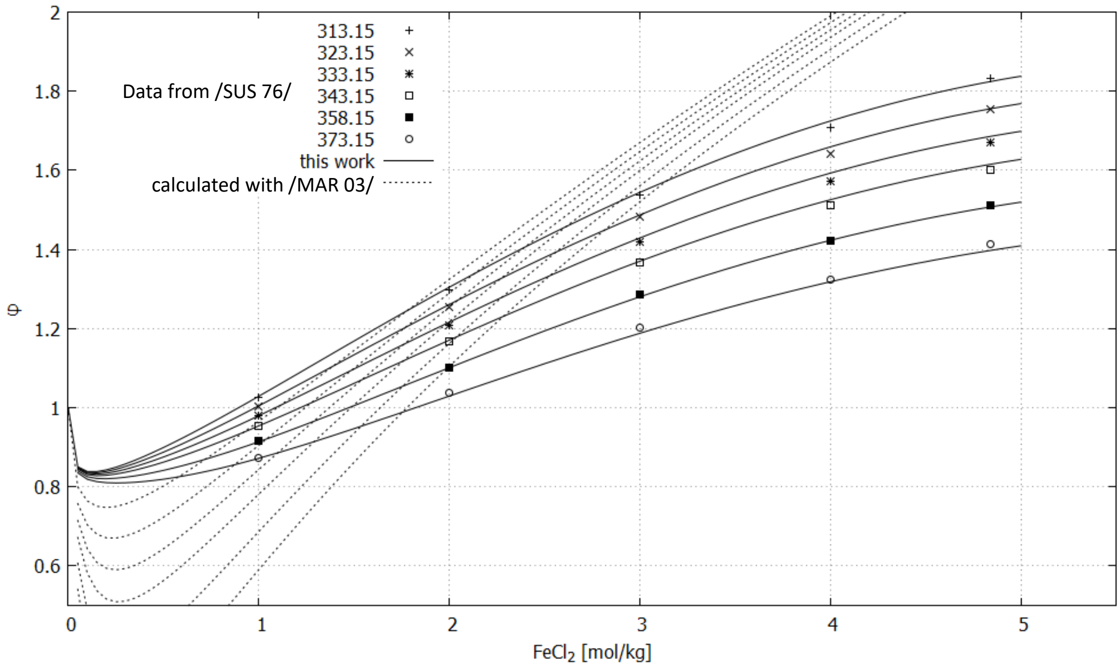


Fig. 3.5 Osmotic coefficients for the system $FeCl_2$ – H_2O at temperatures from 313.15 to 373.15 K

One way out of this predicament could be to restrict the range of validity for a future ferric iron database on physico-chemical boundary conditions of interest and focus new experiments accordingly. Restricting efforts on near-neutral to alkaline conditions could be a first step to eliminate complexes which can be neglected. The important complexes (probably with hydroxide) should be quantified in spectroscopic measurements where the ionic strength along with the presence of other important ligands such as chloride, sulphate, or carbonate is varied. Due to the low solubility of iron under these conditions, the measurement of vapour pressure doesn't seem to be meaningful, while solubility experiments alone seem inappropriate due to long equilibration times, uncertainties with respect to solid phase identification and problems with colloid formation.

If complexes with chloride or sulphate turn out to be unneglectable, published isopiestic data could still prove useful because they could be re-evaluated in conjunction with new spectroscopy data, providing Pitzer coefficients for complex species, instead of free, ferric iron, the relevance of which for nuclear waste scenarios is next to zero. An example is given in the Fig. 3.6; actually, the inclusion of free Fe^{3+} in the speciation model worsens the agreement between calculated and measured solubility at low pH.

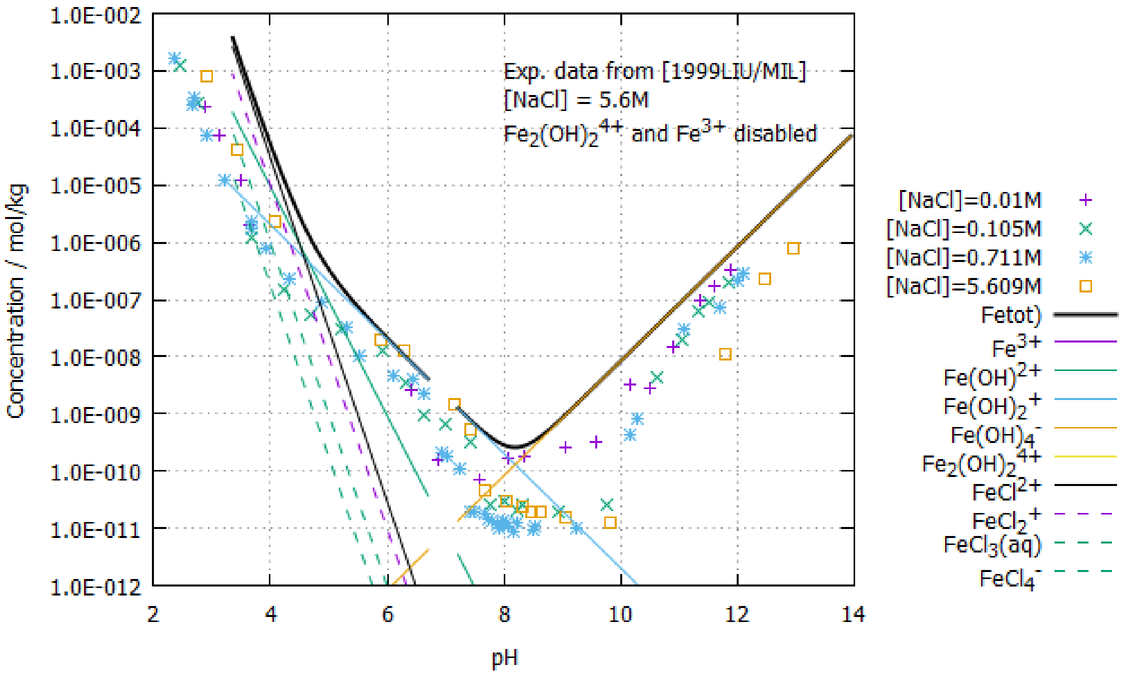


Fig. 3.6 Solubility of Ferrihydrite at 298.15 K. No Pitzer coefficients ferric iron species were applied for this calculation

As to plumbous lead, for near neutral to acidic conditions quite extensive Pitzer models are available. Due to significant complexation with chloride and sulphate, all models are conditional in the sense that any of them has to be adopted “as is” because Pitzer coefficients, stability constants, and solubility constants are mutually dependent. Application of models developed with a focus on seawater on rock salt brines should be avoided due to the formation of $PbCl_4^{2-}$ and the general bias on lower ionic strength conditions.

For neutral to alkaline conditions only few sources exist, and no final judgment is possible as to their applicability to rock salt brines. But there are indications that the strong complexation with chloride prevents the formation of hydroxide complexes up to a certain OH^- concentration, so that the models may be applied to slightly alkaline brines as well. The existence of mixed hydroxide chloride complexes with plumbous lead appears possible but still needs experimental evidence.

Contrary to ferric iron, internally consistent sets of stability constants and Pitzer coefficients were published by several authors, among whom Hagemann provides the largest experimental database to support his model /HAG 99/. Even so, this model has little international recognition because it had never been published in a peer-reviewed paper.

3.8 IAEA Biosphere activities: MODARIA

GRS was observing the work and development in the IAEA project MODARIA (Modelling and Data for Radiological Impact Assessments) to assess their use for future long-term safety assessments in Germany. GRS was only contributing to the work of MODARIA by participating in the discussions but did not perform any modelling work. This overall objective of MODARIA was addressed by undertaking the following activities.

- Defining the key processes that drive environmental change (mainly those associated with climate and climate change) and describing how a relevant future may develop on a global scale. These drivers are quantitative and can be extracted from the existing scientific consensus on global historical climate evolution. The results can be used to describe the future environments, which are called 'reference futures' and 'future variants'. The terminology is designed to show that they are not predictions, but relevant examples that provide valuable input for addressing specific issues in a safety assessment.
- Developing a methodology (as a conceptual framework) for environmental change that is valid on a global scale and showing how that can be downscaled to provide information that may be needed for site-specific assessments.
- Illustrating different aspects of the methodology to a number of case studies (sites) that illustrate the evolution of site characteristics and the implications for the dose assessment models, including the justification of abstraction into simplified assessment-level models. This was intended to address: (a) changes in the potentially affected environment prior to any assessed radionuclide release to the biosphere, and (b) changes occurring after or while releases are assessed to occur, including possible transient effects that may be relevant to resulting potential exposures.

The methodology developed in MODARIA builds substantially on previous assessment work and consolidates a wide range of on-going climate and other international and national level research. It consists of a series of the following sequential steps, called a road map, which are discussed in detail in the different chapters of the final MODARIA report:

1. Determine the geographical context and type of facility: This for example includes information like Host rock type, potential that the site is submerged or glaciated.

2. Determine the timescale over which the assessment is required: Since all types of wastes are considered, different timescales could be relevant.

3. Determine whether new global climate simulations are required or whether results can be utilised from an existing ensemble of simulations.

4. Evaluate whether global climate model outputs and paleo-climatic data are sufficient for informing the required safety assessment and continue with step 6, if found to be true.

5. Select appropriate climate interpolation and downscaling techniques and apply.

6. Model changing landscape using the climate model outputs.

7. Model radionuclide transport through the changing landscape under changing climatic conditions.

8. Evaluate the radiological impacts of the time-dependent pattern of radionuclide concentrations in environment.

Various types of climate model may be used in making projections of future climate on a global basis. These include the more detailed Atmosphere-Ocean General Circulation Models (AOGCMs) and Earth System Models that include the representation of biogeochemical cycles. Alternatively, simplified models may be used for making longer-term projections. Whichever global models or combinations of models are used, the climate outputs provided will be at a rather coarse spatial scale, currently typically 100 km or more. If all that is required for safety assessment is a broad overall projection of future climate changes, then the low spatial resolution of the results may not be an important consideration. Thus, for example, such low-resolution output may be sufficient to establish an associated succession of broadly defined climate domains at a site, together with estimates of the approximate duration of each.

Earth Models of Intermediate Complexity (EMIC) and Atmosphere-Ocean General Circulation Models were presented during the different meetings of the project and also in the final report to predict the influence of the future climate change due to human CO_2 emissions into the atmosphere on the landscape and the deep geological repository. The method was applied exemplarily to a number of case studies (sites), illustrating the evolution of site characteristics and the implications for the dose assessment models, including the justification of abstraction into simplified assessment level models. This may address: (a) changes in the potentially affected environment prior to any assumed radionuclide release to the biosphere, and (b) changes occurring after or while releases are assumed to occur, including possible transient effects that may be relevant to resulting potential exposures.

The use of a traceable and systematic approach to making projections of long-term climate and landscape change, based on the latest scientific understanding, helps to build confidence in the resulting safety and performance assessments. The road map developed within MODARIA has drawn on experience and expertise from a range of countries and contexts to establish an approach that may be applied consistently across different radioactive waste disposal programmes. Indeed, updated projections of global climate for a wide range of different CO_2 emission scenarios provides a suite of global climate projections that may be used as a starting point for assessments and thus encourages consistency in the treatment of long-term environmental change across different national radioactive waste disposal programmes.

The report is expected to be finished and the report to be published by IAEA in 2018 and a summary was presented in /LIN 18/. It will have to be discussed than, if the method developed in the MODARIA project should be exemplarily applied to a generic repository site in Germany.

4 Selected topics

4.1 Bentonite re-saturation - limited access to water

4.1.1 Motivation

The dynamics of water uptake in terms of the evolution of the water content distribution inside a bentonite buffer have already been extensively tested in the laboratory e. g. /BÖR 84/, /KRÖ 04/, /FRA 17/. All these experiments have at least the potential to show the water uptake dynamics in great detail. However, they all allowed unimpeded access to water (UA) for the bentonite meaning that the water uptake rates are exclusively controlled by the ability of the bentonite to take up water.

Under in-situ conditions, by contrast, comparatively low flow from the rock can be found. The related flow rates show that a potential host rock for a nuclear waste repository will initially not provide as much water as the bentonite would take up under UA-conditions. The same applies to smaller fractures with comparatively low transmissivity. In this case a limited water supply rate (LWSR) for the bentonite buffer can be envisaged. Detection of a detailed transient water content profile under in-situ conditions is not possible, though, due to the spatial requirements of the measuring equipment. The water uptake dynamics of a bentonite buffer under LWSR-conditions were thus not really known. Chapter 4.1.2 summarizes the work to provide detailed data about the water uptake dynamics of compacted bentonite under LWSR-conditions which is described in detail in /KRÖ 18/.

4.1.2 Finding a suitable test-setup

The planned test series had been envisaged as a supplementary experiment supporting the Buffer-Rock Interaction Experiment (BRIE) at the HRL Äspö in Sweden /FRA 17/ at an early phase. It was designed as a standard uptake test connecting a water reservoir with the compacted bentonite with the modification that the water had to pass a piece of Äspö granite before reaching the sample (see Fig. 4.1). By this modification the water uptake was supposed to be sufficiently impeded. The granitic disc, however, proved to be too watertight for this experiment. Even after 3 weeks of contact with a fully saturated granite disc the bentonite showed no response in terms of increasing water content. Looking for a suitable artificial porous material also glass sinter plates were tested. In this case the plates with the lowest permeability were still too permeable, though, to pose a serious impediment for the water from the reservoir.

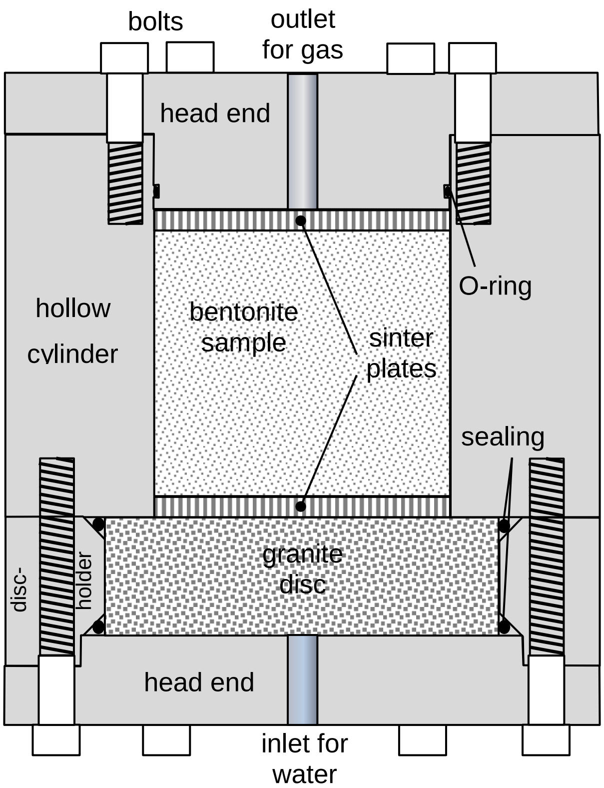


Fig. 4.1 Test cell for inflow reduction by low permeable porous material

Instead of investing further in the time-consuming search for a suitable flow impeding porous material the test concept was changed. As with the previous concept a series of tests with different test durations was planned to show the different stages of re-saturation. The test cell remained basically the same as illustrated in Fig. 4.1 without the granitic disc. Instead of impeding the inflow rate for the bentonite by a hydraulic resistance to flow it was tried to control the flow rate directly. The flow rates for a bentonite sample with a diameter of 50 mm required to achieve LWSR-conditions lie in the range of 0.01 ml/h to 0.03 ml/h. In order to distribute the water equally over the whole face of the sample it was positioned over a free water surface that would rise according to the target inflow rate for the bentonite (see Fig. 4.2). In this set-up the bentonite is not permanently in contact with water. The water table in the bowl rises according to the continuous flow from the pump. Upon reaching the bentonite the sample sucks up water thereby lowering the water table and interrupting water uptake. These discontinuities were considered tolerable, though, in the light of test durations in the order of weeks.

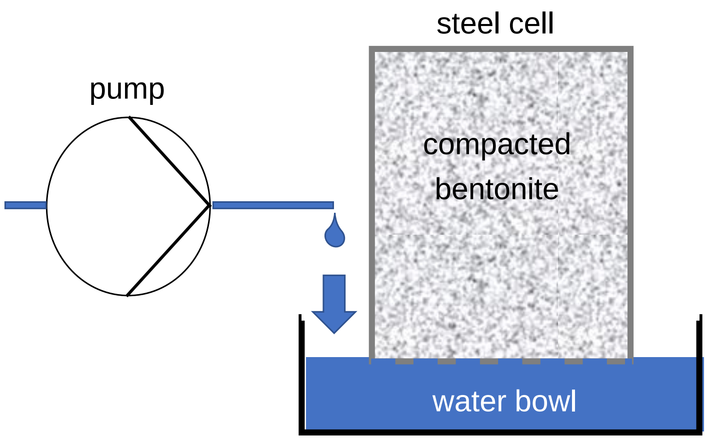


Fig. 4.2 Test principle for direct inflow control via water bowl

Two major practical problems arose with this test set-up that could eventually not satisfyingly be solved: determining the time of the first contact with water and preventing or quantifying evaporation from the water bowl. In the end the water was directly injected from below into the test cell that had been modified according to

Fig. 4.3. In order to distribute the water equally over the whole face of the sample sinter plates were used.

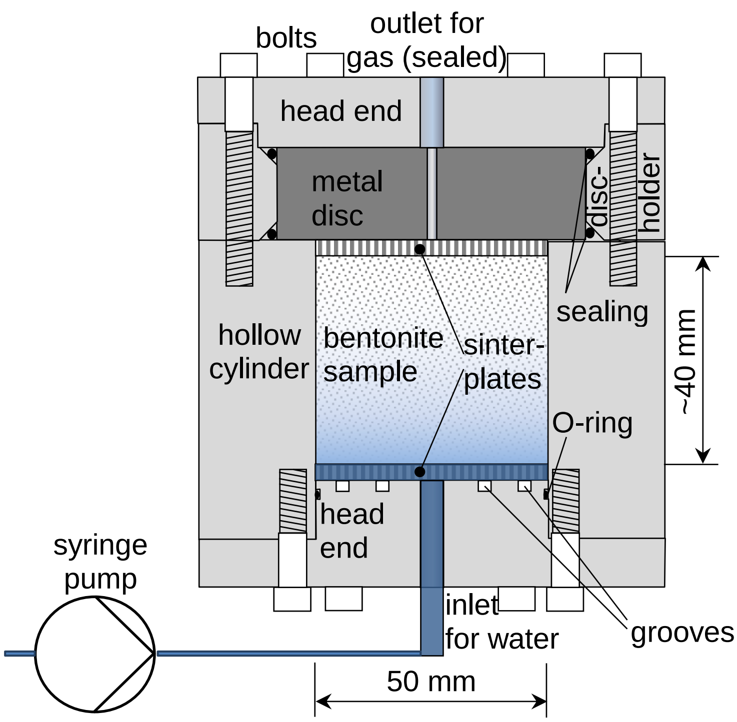


Fig. 4.3 Final test setup

4.1.3 Test program and modelling prerequisites

Two series of water uptake tests were performed. In one series the duration of the individual tests was fixed to approximately one week and the inflow rate was varied between 0.01 and 0.04 ml/h. For comparison, also a test with an inflow rate of 0.05 ml/h over two weeks is included here. In the second series the inflow rate was set to 0.02 ml/h and the test duration was varied amounting to 1, 2, 3, 4, 7, and 9 weeks. The tests were performed with MX-80 bentonite at a target density of 1450 kg/m³ being wetted by a solution typical for the Äspö HRL.

In parallel, the concept of the extended vapour diffusion (EVD) model for water uptake by compacted bentonite under confined conditions /KRÖ 11/ had been advanced on a theoretical basis to cope with LWSR-conditions. Appropriate formulations were derived /KRÖ 17/ and implemented in the referring code VIPER. The combination of theoretical considerations, realisation as a code and experimental inspection allowed for checking the new model concept qualitatively as well as quantitatively and thereby for qualifying the advanced code VIPER.

4.1.4 Results

The results of the laboratory tests varying the inflow rate as well as the results of the related model calculations are superimposed in Fig. 4.4. The calculated water content for the three lowest inflow rates matches the measurements satisfyingly well and is thus corroborating the theoretical considerations concerning the new model developments for LWSR-conditions. The overall characteristics of these water content curves appear to be consistent with a diffusion-like water migration process. Contrary to water uptake under UA-conditions where the water content at the inflow boundary shows its maximum value from the beginning on the present measurements show water content distributions whose boundary values increase with the inflow rate. The highest value along with the highest gradient can be found at the inflow boundary and it decreases exponentially with distance from this boundary.

In case of the inflow rate of 0.04 ml/h, however, an overly high water content along with a steep downwards gradient can be observed close the water inlet at the expense of the water content further into the sample. This high value is not in line with the remaining water content distribution. It appears that the forming of the fully saturated zone at the bentonite-water contact that had been observed in earlier water uptake tests under

UA-conditions (e. g. /KRÖ 04/) begins to take hold. This conclusion is corroborated by an early test with an inflow rate of 0.05 ml/h over two weeks where the water content in the first two millimetres exceeds even the theoretical water content at full saturation.

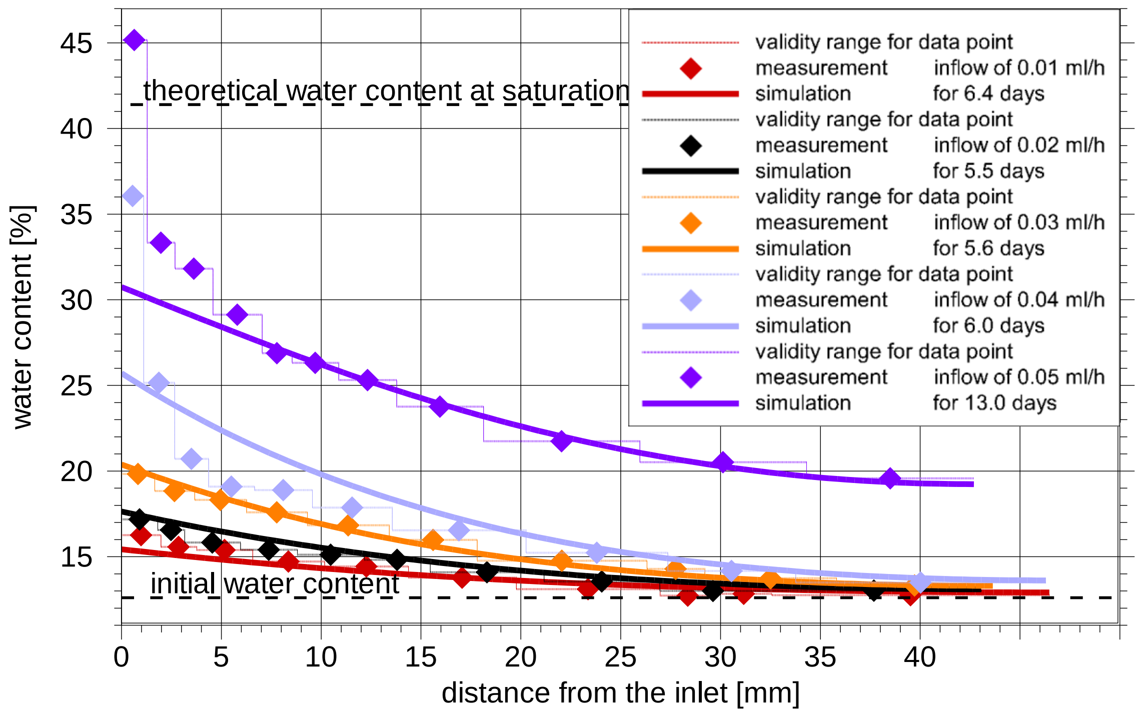


Fig. 4.4 Measured and calculated water content distributions varying the inflow rate

Measurements and model calculations for an inflow rate of 0.02 ml/h for varying periods of time as depicted in Fig. 4.5 point in a similar direction. For the tests lasting up to four weeks basically an upwards shift of the water content curve can be seen in model and measurement, again confirming the theoretical considerations concerning uptake under LWSR-conditions. Apparently, the diffusive water flux along the sample axis distributes the inflowing water more or less equally over the whole sample length. Accumulation of water at the inflow boundary is therefore not possible during this period of time.

However, already in the measurements after four weeks there is a slightly too high value at the inflow boundary that does not quite fit the trend of the rest of the water content distribution. This deviation is more pronounced in the curve for 7 weeks test duration after which the full saturation of the interlamellar space is reached. For orientation this value is indicated in Fig. 4.5 for the two longest lasting tests by two dashed lines. Continuing the test for another two weeks produces even a peak at the boundary that exceeds the theoretical water maximum content. This value is indicated in Fig. 4.5 as well in the same way.

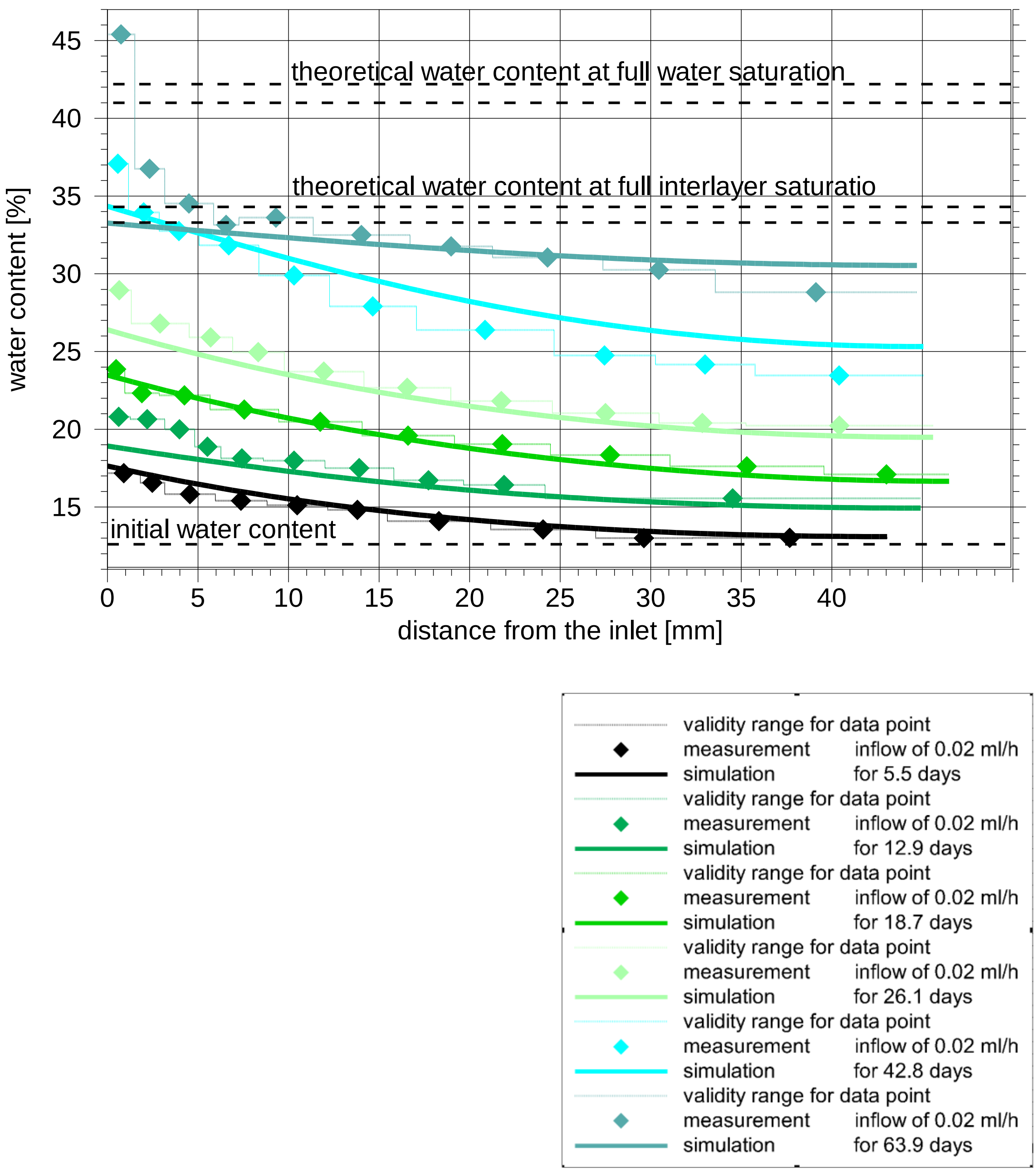


Fig. 4.5 Measured and calculated water content distributions varying the running time

The comparison of measurement and simulation for each single test shows in some cases potential for a better fit. As an ensemble, though, the calculated water contents match the measured ones fairly well thereby confirming the assumptions of the EVD-concept in general and the considerations about the specific aspects of uptake under LWSR-conditions in particular.

4.1.5 Conclusions

Detailed data about the water uptake dynamics of compacted bentonite at the bentonite-rock contact under a limited water supply rate from the rock (LWSR-conditions) have been gathered experimentally. The evolution of the water content was measured varying the inflow rate over a fixed period of time as well as the running time of the tests at a fixed inflow rate. The obtained water content distributions are characteristic for diffusive water migration.

The evolution of the water content distribution under LWSR-conditions is decidedly different from the evolution previously explored in other tests under unimpeded access of the bentonite to water (UA-conditions). The fully saturated zone observed under the latter conditions does not appear during the comparatively early stages of the present tests. It seems to develop later on, though.

Modelling of water uptake under LWSR-conditions has been made possible by advancing the extended vapour diffusion (EVD) model conceptually and numerically. After calibration it was thus possible to compare experimental and numerical results quantitatively. Matching numerical and test results to a reasonable degree was possible within acceptable parameter ranges and with only one parameter set, thereby backing up the assumptions of the EVD-concept in general and the considerations about the specific aspects of uptake under LWSR-conditions in particular.

Modelling based on the EVD-approach indicates that the water migration processes adopted and qualified for UA-conditions also explain the uptake dynamics under LWSR-conditions. Conceptualisation, modelling and measurements thus provide a consistent framework for describing the re-saturation of a bentonite buffer at repository-relevant flow rates. It has to be kept in mind, though, that after a significant period of time the measurements indicate an additional process close to the inflow boundary that is not yet captured in the advanced framework of the EVD-model.

4.2 Bentonite re-saturation – non-isothermal water uptake

4.2.1 Motivation

Laboratory water uptake tests had been commenced in the framework of the previous project "Scientific basis for a safety case of deep geological repositories" (WiGru-6) /NOS 12/. The motivation given there is still valid and was summarized as: "Discussions in the TF EBS[3] had shown that there is no conclusive experimental evidence about the steady-state conditions after a non-isothermal re-saturation. Characteristic for the present state of knowledge are the two laboratory experiments performed by CEA /GAT 05/ and CIEMAT /VIL 05/ that formed the basis for the first two test cases[4] in the TF EBS. The two tests of CEA indicate an evenly distributed water content distribution at a level related to a fully vapour saturated pore atmosphere. However, both tests were terminated before reaching such a state. Contrary to these results the test of CIEMAT showed after about a year of running the experiment no changes in the relative humidity, which was considerably lower at the heated side than at the cool side of the sample. Similarly, ambivalent are the results of the mock-up test in the Febex-project (e. g. /SAN 06/). It is thus unclear whether the re-saturation models are able to describe the steady-state conditions correctly. To answer this question with a view to hydraulic conditions a laboratory experiment was devised."

1.1.1. Test set-up and procedure

The design of the experiment had in principle been quite similar to the set-up used previously for isothermal water uptake tests in the framework of the EBS-project /KRÖ 04/. However, because of the superimposed temperature gradient a different kind of measuring cell was required. It was imperative to cut and preserve the specimen very fast in order to avoid evaporation of water from the heated slices. Therefore, a set of 10 bolted plastic rings replaced the steel cylinder as shown in Fig. 4.6. The cylindrical bentonite samples had a diameter of 5 cm and a length of 9.5 cm. Pre-tests were performed to optimise the experimental set-up minimising lateral heat loss and thereby deviations of the temperature profile from a linear temperature gradient along the sample axis.

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[3] Task Force on Engineered Barrier Systems

[4] Presently referred to as "Task 1 – Laboratory tests"

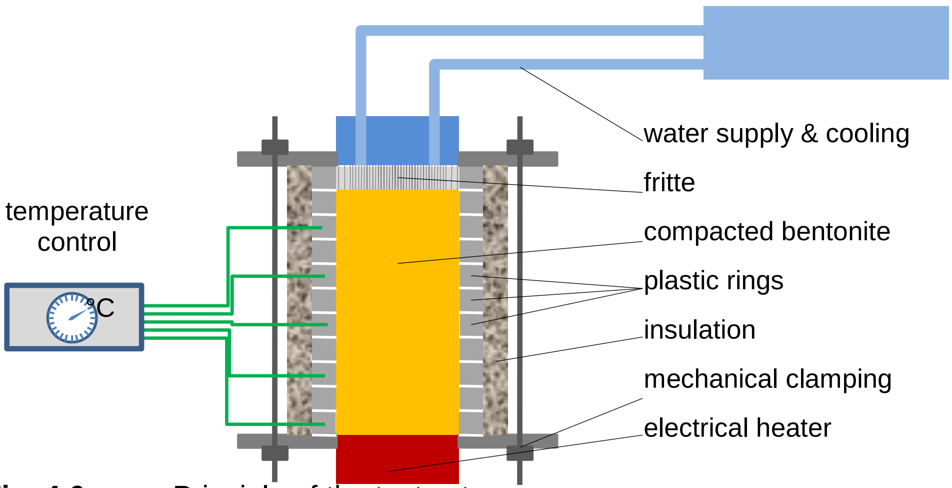


Fig. 4.6 Principle of the test set-up

Four cells were run in parallel. Each of the cylindrical samples was hydraulically loaded from one planar side and thermally loaded from the opposite side. After a pre-defined period of time each individual test was terminated and the water content distribution over the sample determined. After cleaning the cell, a new sample was installed and the test was re-run for a different period of time. Especially for short running periods the tests were repeated to evaluate their reproducibility. All in all, 33 tests were performed.

4.2.2 Test history

At the end of the project WiGru-6 the tests had been running for up to 72 weeks. Nevertheless, neither the water content evolution nor the inflow rate showed signs of reaching steady-state conditions. Continuation of the experiment especially of the already long running tests was therefore recommended and eventually granted with the present project.

Particularly long durations were envisaged for further tests. It turned out, though, that the total amount of water seemingly taken up by the samples exceeded the theoretical maximum water uptake capacity of the samples significantly. Leakage between rings of the test cells, lifted apart as a consequence of the exerted swelling pressure of the wetted bentonite was suspected. The test set-up was therefore revised and strengthened where possible. Seven long-term tests were performed with the new set-up. It turned out, though, that further leakage could not entirely be prevented by the cell improvement.

To identify by running time each test will be labelled in curly bracket by the referring test duration where “D” stands for days and “W” for weeks. Where tests had been repeated the sequence is defined by a following lowercase letter such as {2 D a} or {16 W b}. The sequence of the tests is tabulated in Tab. 4.1.

Tab. 4.1 Sequence of the individual tests

Begin	End	Test abbreviation	Remark
15.6.10 11:30	17.6.10 12:00	2 D a	
16.6.10 10:30	17.6.10 11:00	1 D a	
17.6.10 14:00	21.6.10 14:00	4 D a	
23.6.10 10:00	30.6.10 10:30	7 D a	
24.6.10 10:15	8.7.10 7:30	2 W a	
6.7.10 11:00	19.6.13 16:00	154 W	planned as 208 W a
8.7.10 10:00	28.10.10 10:00	16 W a	
7.7.10 15:30	23.11.11 12:00	72 W	
13.7.10 9:30	14.7.10 10:00	1 D b	
20.7.10 9:30	22.7.10 10:00	2 D b	
2.8.10 11:00	2.8.10 11:00	4 D b	
16.8.10 11:00	16.8.10 11:00	7 D b	
17.8.10 11:30	12.10.10 10:00	8 W a	
19.10.10 9:45	9.2.11 10:00	16 W b	
4.11.10 9:00	16.6.11 9:00	32 W a	
15.2.11 10:30	16.3.11 9:50	4 W a	
30.3.11 9:45	20.6.12 10:00	64 W	
21.6.11 11:00	19.7.11 11:00	4 W b	
26.7.11 11:30	9.8.11 12:00	2 W b	
16.8.11 10:00	11.10.11 12:00	8 W b	
18.10.11 10:00	11.2.15 16:00	173 W	planned as 208 W b
29.11.11 10:30	30.11.11 11:00	1 D c	
1.12.11 10:15	27.11.13 16:00	104 W a	
26.6.12 10:00	28.6.12 10:00	2 D c	
10.7.12 9:37	11.7.12 10:00	1 D d	
17.7.12 9:31	11.2.15 16:00	134 W	planned as 156 W a
3.4.14 12:30	28.5.14 16:00	8 W c	
22.7.14 9:15	13.11.14 16:00	16 W d	
23.7.14 0:00	21.7.16 0:00	104 W b	
17.12.14 0:00	13.12.17 0:00	156 W b	
10.3.15 0:00	23.3.18 0:00	160 W	planned as 156 W c
26.03.15 15:05	6.11.15 0:00	32 W b	
26.3.15 15:25	1.2.17 0:00	96 W	

4.2.3 Characteristic material data

Characteristic values for the experiment were determined as a mean over 26 single tests. The data allowed conclusions concerning the uncertainties introduced by the manufacturing process. By this measure three samples with uncharacteristic deviations were identified that had produced misleading results. The related tests were subsequently excluded from further evaluation. The data from the remaining samples are compiled in Tab. 4.2 together with the referring maximum and minimum values as well as the standard deviation.

The dry density was derived from drying the bentonite discs that had to be cut from the sample with a scraper. This is a rough method of obtaining discs leading to over- or underestimation of the bentonite mass related to a ring. The derived dry densities were therefore subject to uncertainties that should, however, have been averaged out over the sample.

Tab. 4.2 Characteristic values for the experiment

Quantity	Unit	Maximum	Minimum	Mean	Standard deviation
Sample height	[cm]	9.70	9.45	9.54	0.06
Sample diameter	[cm]	5.00	4.99	4.99	0.00
Sample volume	[cm³]	189.70	184.81	186.74	1.11
Dry mass	[g]	280.81	263.34	268.51	3.62
Initial mass (air dry)	[g]	306.44	291.15	296.86	3.56
Initial water content	[-]	11.23	9.13	10.56	0.40
Dry density	[g/cm³]	1.505	1.407	1.438	0.021
Initial density	[g/cm³]	1.643	1.555	1.590	0.020
Dry porosity	[-]	0.494	0.458	0.483	0.007
Initial porosity	[-]	0.346	0.313	0.331	0.008
Water uptake capacity	[g]	92.76	85.52	90.16	1.66
max. water content	[%]	35.10	30.46	33.59	0.99

4.2.4 Results for the original test set-up

4.2.4.1 Temperature distribution

All tests cells were equipped with at least one sensor for the top and for the bottom ring to monitor temperature. In one cell even each ring contained a temperature sensor to check on the temperature gradient along the sample axis. The results for different tests performed with this cell are compiled in Fig. 4.7. The curves indicate a reasonable approximation of the intended linear temperature gradient.

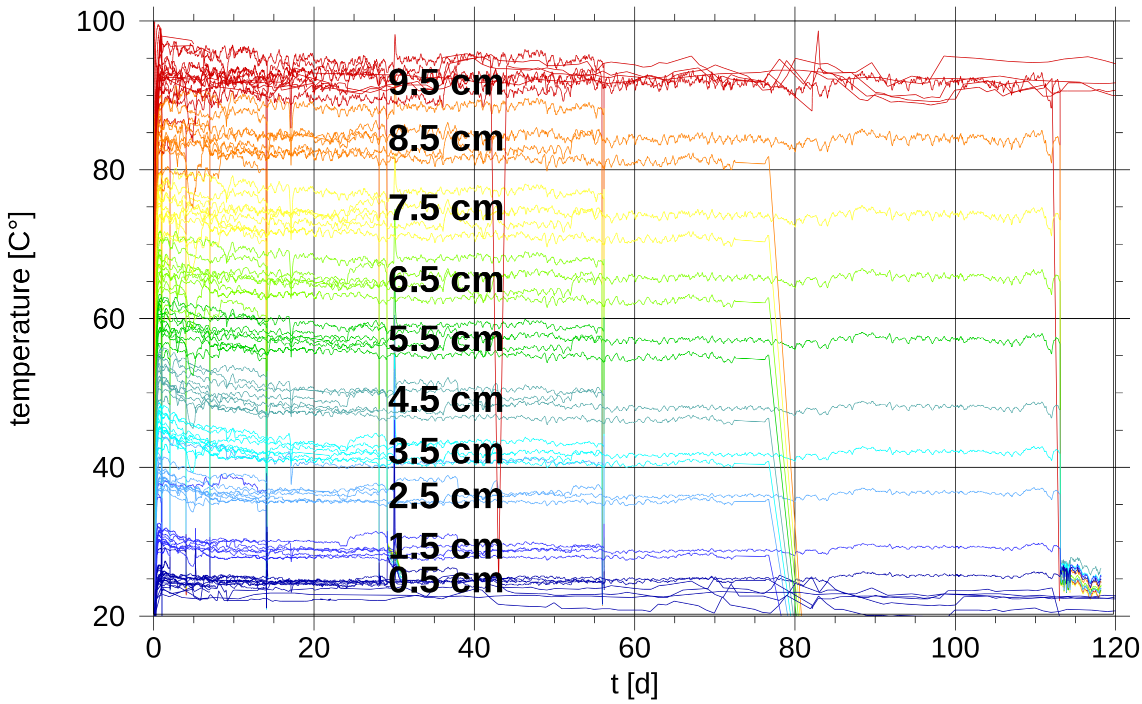


Fig. 4.7 Temperature level and evolution during uptake tests until 16 weeks

4.2.4.2 Reproducibility of the tests

Several tests were repeated to check the uncertainty to the derived water content distributions. In order to minimize the resulting impediments of the whole experiment this was done for tests up to a running time of 16 weeks. The results from tests with the same running time were averaged.

A comparison of the related 160 data points yields the following statistics concerning the deviations Δw from the mean water content value:

– 2 cases with $\Delta w > 0.02$

– 12 cases with 0.01 < Δw < 0.02
– 146 cases with Δw < 0.01

Based on these statistics the tests are considered to be fairly well reproducible. Further control tests were therefore not deemed necessary. However, if leakage occurred during the first 16 weeks this result implies also that the referring experimental flaw would also have been reproducible.

4.2.4.3 Dynamics of the water content distribution

All water content distributions measured with the original test set-up are shown together in Fig. 4.8. They are constructed by linear connections of the single water content values that are representative for the referring bentonite discs and are assigned to the barycenter of these discs.

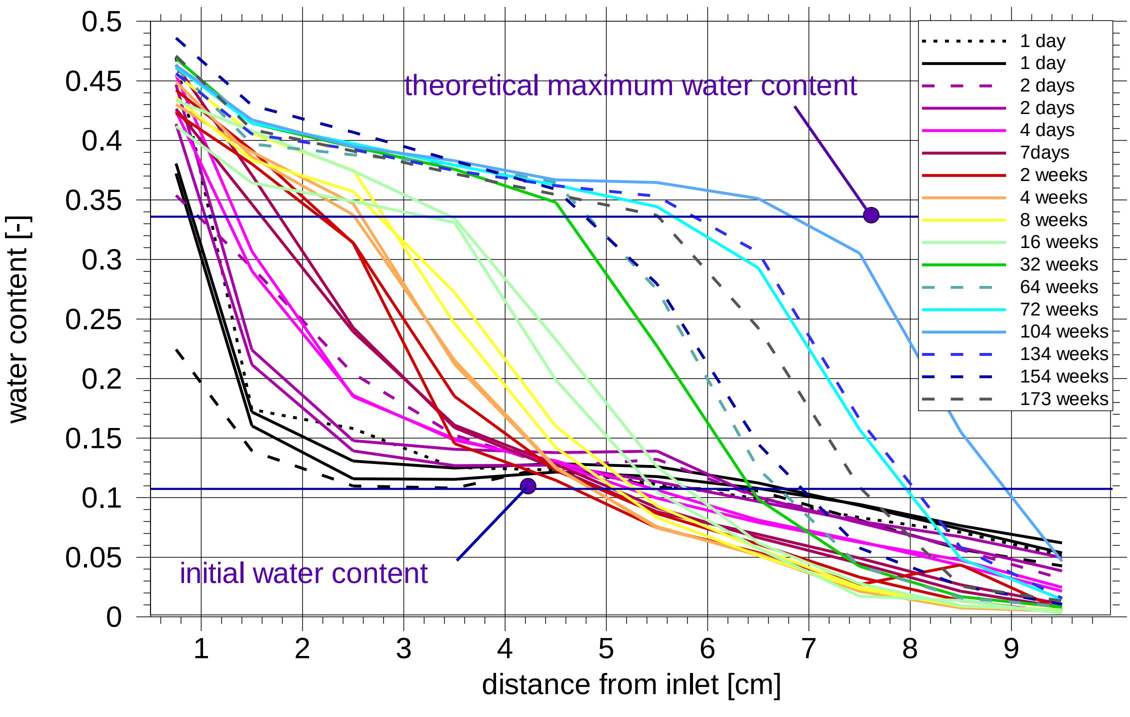


Fig. 4.8 Dynamics of the water content distribution; dashed lines represent problematic results

Some distributions in Fig. 4.8 are plotted with dashed lines to indicate problematic tests that are not taken into further consideration. This concerns tests {1 D a}, {1 D c}, and {2 D a} because of non-conformance with the average samples characteristics (cf. section 0) and tests {64 W}, {134 W}, {154 W}, and {173 W} because the position of the wetting front is not consistent with less long running tests and strongly suggest leakage during the test. However, as {72 W}, and {104 W} were prematurely terminated because of apparent discrepancies between measured water inflow and theoretical maximum water content it cannot be excluded that those tests are also influenced by leakage. It must therefore be conceded that even less long running tests might have been affected.

4.2.4.4 Water content at the water inlet

From theory /KRÖ 11/ and prior experiments /KRÖ 04/ it was expected that the water content at the water inlet reaches quickly a constant value according to full saturation. This maximum water content can be calculated from the dry density. Taking the mean values for the experiment from Tab. 4.2 yields a theoretical maximum water content of about 33.6 %.

Measured, though, were water contents ranging from 41 % to 47 %, not counting the test results for one day running time. These agree very well with each other but show only a water content of 37 % and 38 %, respectively. Two conclusions arise from these observations. Firstly, like in the isothermal uptake experiment described in /KRÖ 04/ the initial fast water uptake appears to result in significant local swelling within the confinement of the test cell. Secondly, the somewhat lower water content values for tests {1 D b} and {1 D d} might indicate that most of the fully saturated zone is formed quite quickly but the process as a whole seems to be completed only after two days.

4.2.4.5 Characteristic phases during evolution of the water content distribution

The initial phase of water uptake and moisture re-distribution can well be explained on the basis of Fig. 4.9. Here the mean water content distribution for running times of 1, 2 and 4 days including an error bar indicating the differences between tests of the same running time are depicted. During the first 4 days there is clearly little interaction of the drying at the hot end of the sample and the wetting at the cool end. But it can also be seen that the wetting affects the sample only to a limited depth. In case of isothermal tests under similar conditions the wetting front did also not reach beyond 4 cm into the sample after 4 days /KRÖ 04/. In contrast, the moisture re-distribution due to heating appears to affect the whole sample length towards the wetting front. At 4 days running time wetting and drying lead more or less to the well-known diffusion-like water content distribution.

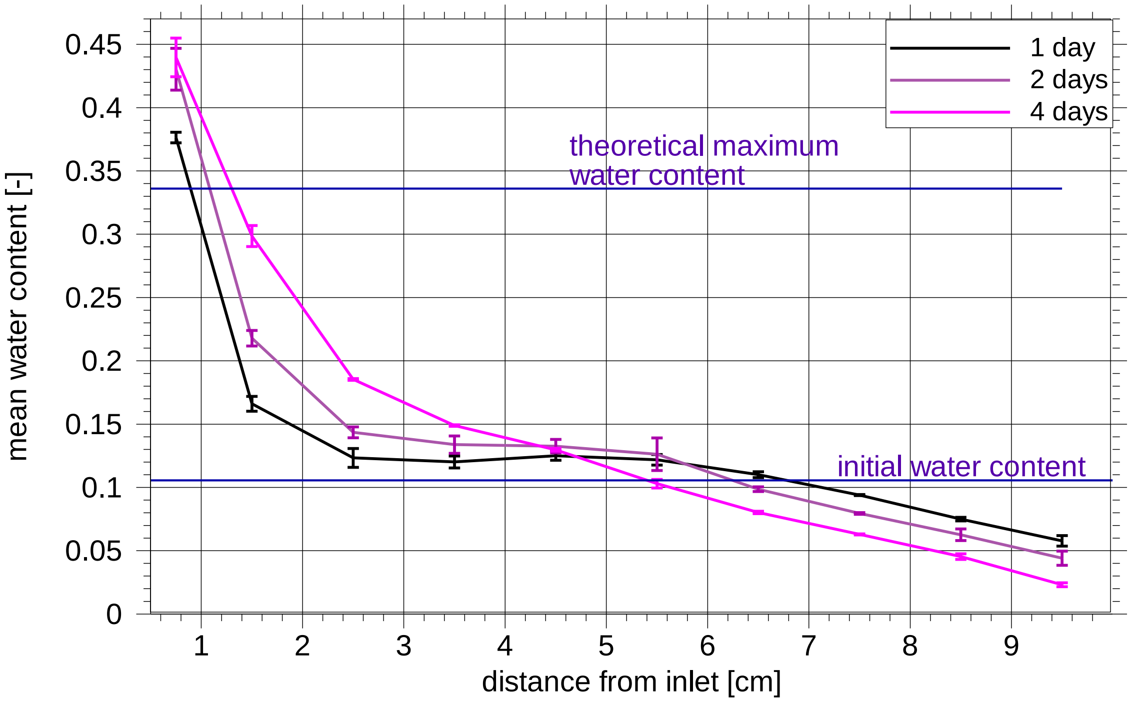


Fig. 4.9 Mean water content distributions for running times of 1, 2 and 4 days

After 7 days, however, the water content distribution begins to develop an inflection point leading to a considerable steepening of the wetting front as shown in Fig. 4.10. After 16 weeks the front has a length of only about 2 cm covering a drop from 35 % down to 10 % water content. Meanwhile, the water content in the dried-out range at the heater does not change significantly.

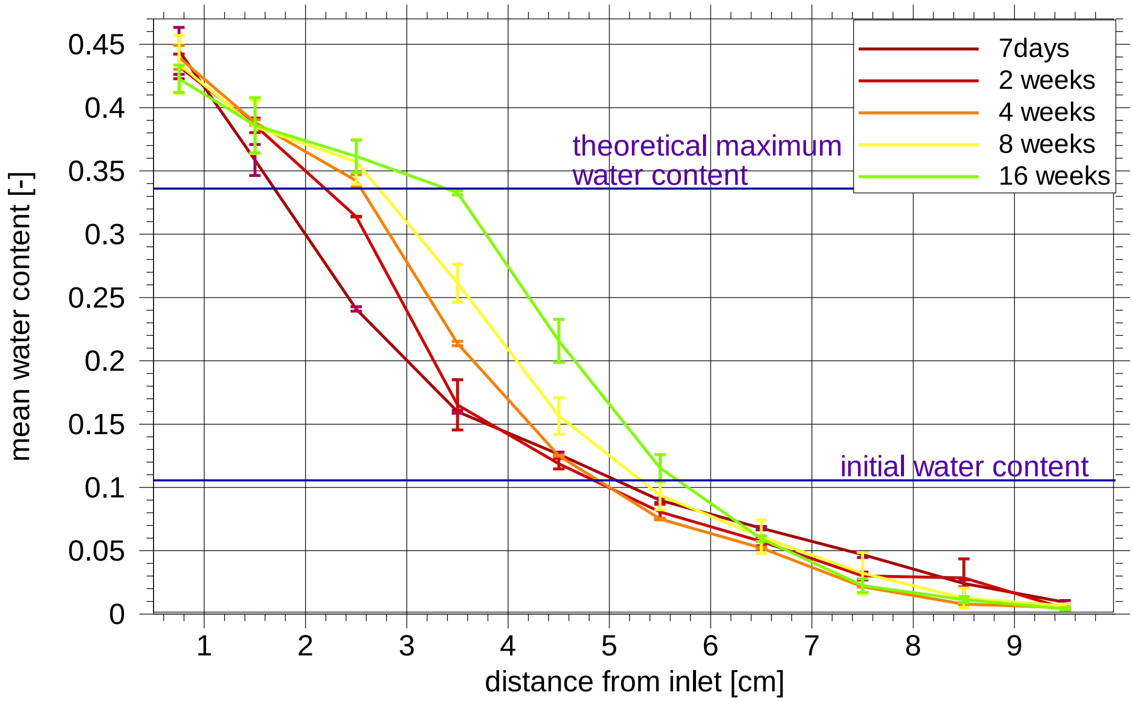


Fig. 4.10 Mean water content distributions for running times of 1 to 16 weeks

A compilation of all (mean) water content distributions is given in Fig. 4.11. Most prominent is the fact that the steep wetting front developed between 2 and 8 weeks running time is preserved over the rest of the test series. The upper end of the front relates in all cases closely to the theoretical maximum water content. After about 100 weeks the wetting front seems to hit the heated side of the sample, beginning to increase the water content at that location.

Also remarkable is the spreading of the zone with water contents exceeding the theoretical maximum value. This is in clear contrast to the isothermal tests where this zone was restricted to the first 4 mm over the whole experimental period covering 186 days /KRÖ 04/. Measurement errors as indicated in Fig. 4.9 as well as in Fig. 4.10 are too low to explain this phenomenon. Furthermore, it has to be noted that the water content distribution appears to converge in the range of very high values.

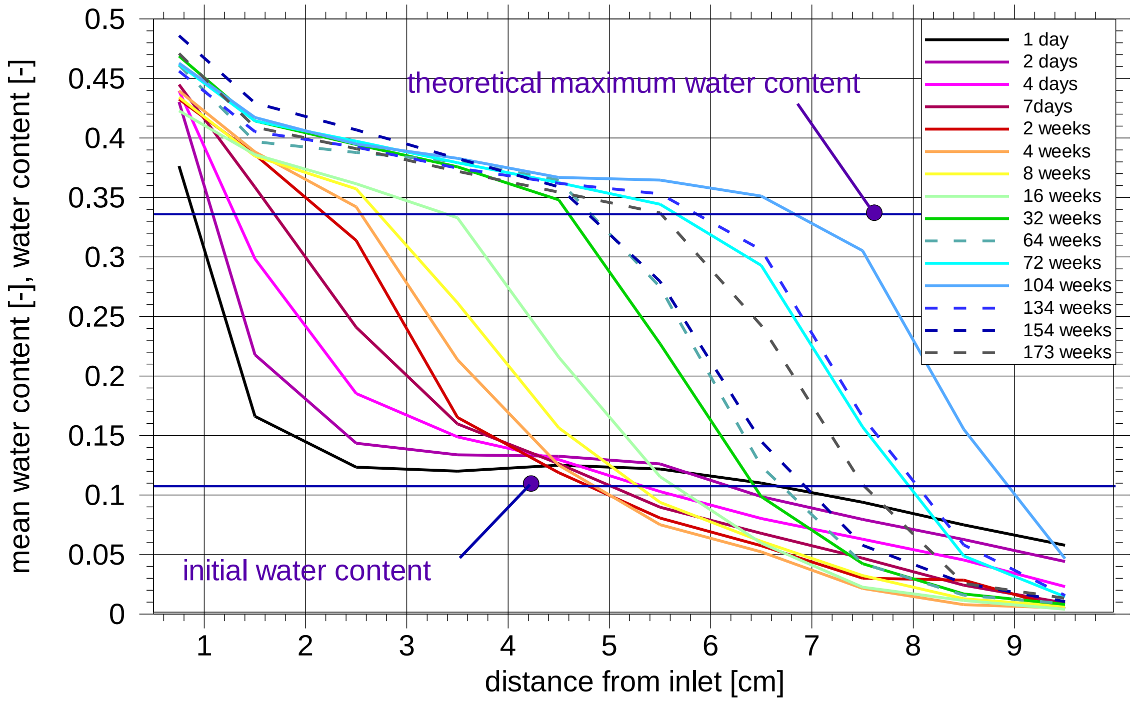


Fig. 4.11 Mean water content distributions for all running times

4.2.4.6 Water uptake from the reservoir

The cumulated amount of water taken up from the reservoir was monitored. The resulting curves appear to be separated by offsets that are most probable the consequence of the difficulties monitoring the water uptake during the very first stage of each test. For comparison these offsets were determined and discounted individually for each curve. The water uptake curves for the first 14 days are depicted in Fig. 4.12. They show a characteristic course that is consistent with the water uptake rates from other experiments.

Later on, though, the curves seem to converge to an almost linear dependency as shown in Fig. 4.13. Furthermore, some of the samples seem to take up spontaneously quite large amounts of water after which uptake returns to the previously shown evolution dynamics.

This behaviour indicates an early deviation from the expected water uptake dynamics. The linear trend in water uptake corroborates the notion of leakage. Leakage might easily lead to steady-state conditions where water uptake from the reservoir is in in dynamic equilibrium with the unplanned outflow. The erratic jumps in the uptake curves might be a consequence of the progress of the fully saturated zone and the related structural changes in the bentonite due to swelling. This could either lead to additional leaks along the sample or might affect the pathway between inflow and the leak(s).

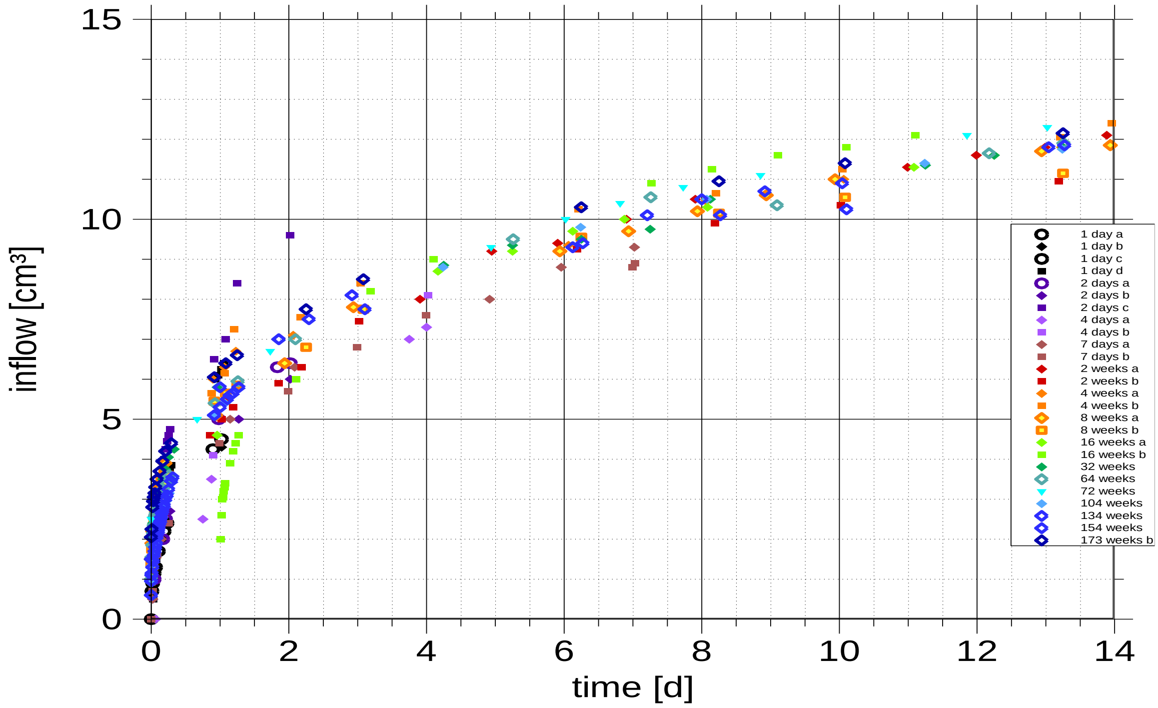


Fig. 4.12 Accumulated water mass for 26 tests during the first 14 days (old set-up)

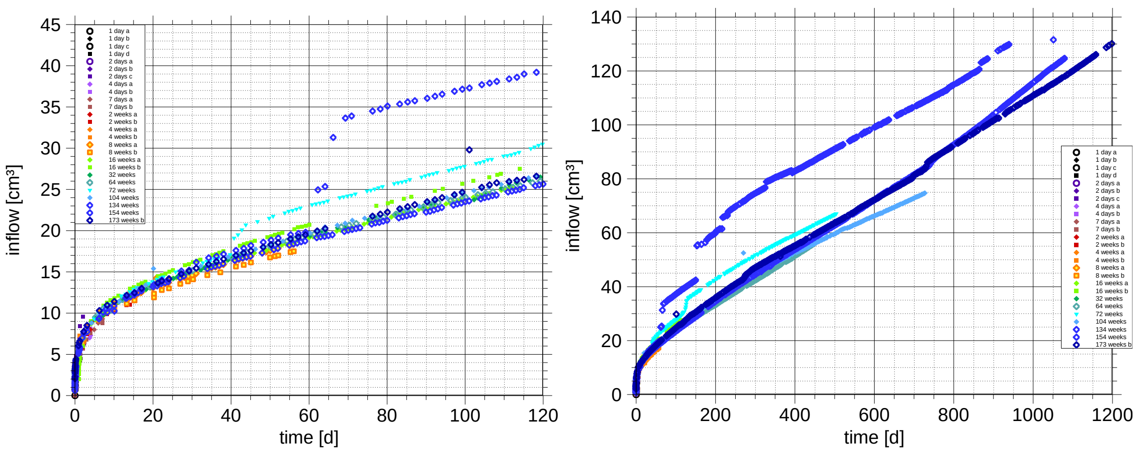


Fig. 4.13 Accumulated water mass for 26 tests during the first 120 days (left) and 600 days (right) (old set-up)

4.2.5 Results for the improved test set-up

Tests {8 W c}, {16 W d}, {32 W b}, {96 W}, {104 W b}, {156 W b}, and {160 W} were performed with the improved test set-up. Fig. 4.14 shows the determined water content distributions.

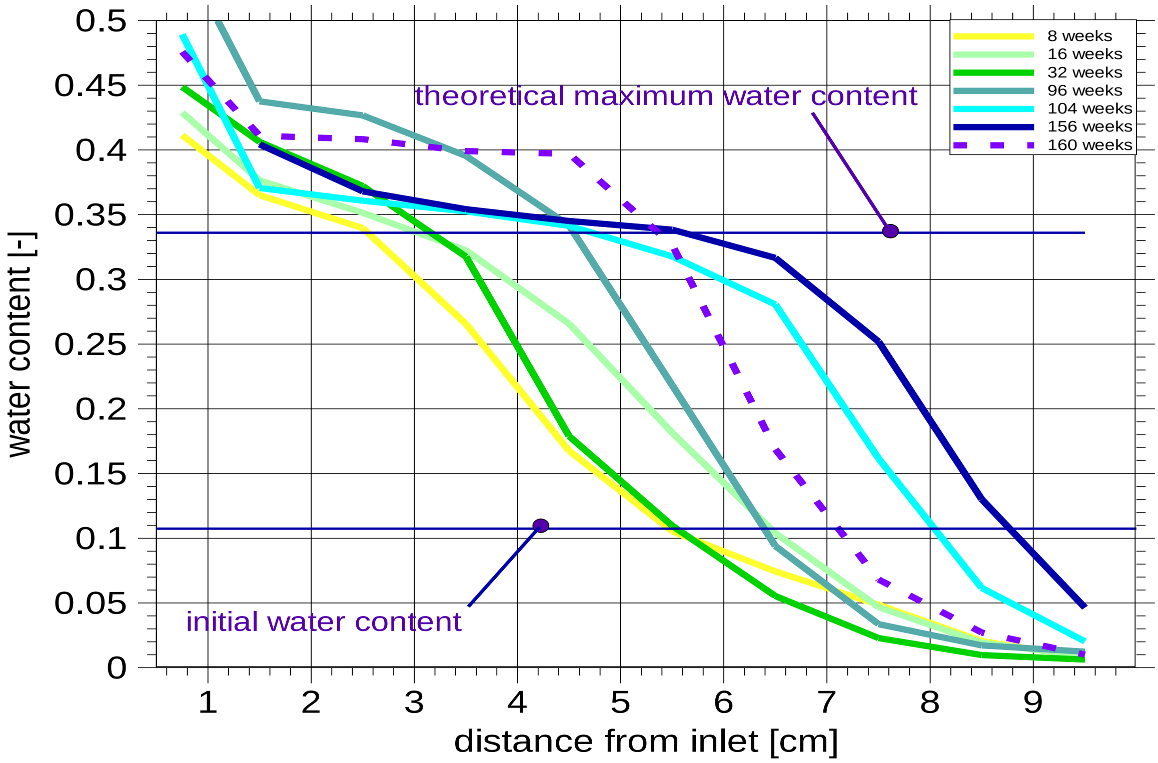


Fig. 4.14 Water content distributions determined with the new test set-up

The water content curves for the shortest running times, namely 8 and 16 weeks, look qualitatively different from the longer running tests in that they show a much smoother wetting front. The others have again the steep wetting front and show in general the same characteristics as those curves obtained with the old test set-up. It can thus be speculated that the improved set-up withstood the developing swelling pressure better than the original set-up but possibly only to a certain extent. After development of a certain swelling pressure leakage apparently occurred again. This view is corroborated by the fact that the water content distribution of test {160 W} reaches significantly less deep into the sample than that of test {104 W}.

Further evidence comes from Fig. 4.15 depicting exemplarily the water uptake after 120 and 1200 days, respectively. During the first 120 days the water uptake curves for tests {8 W c}, {16 W d}, {104 W b}, and {156 W b} look quite consistent with the idea of diffusion-like water transport in the bentonite. Later on, however, the curves converge towards a rather constant uptake rate that in case of tests {104 W b} and {156 W b} even increases seemingly spontaneous. Also, a jump in the accumulated mass taken up can be observed again at test {96 W}.

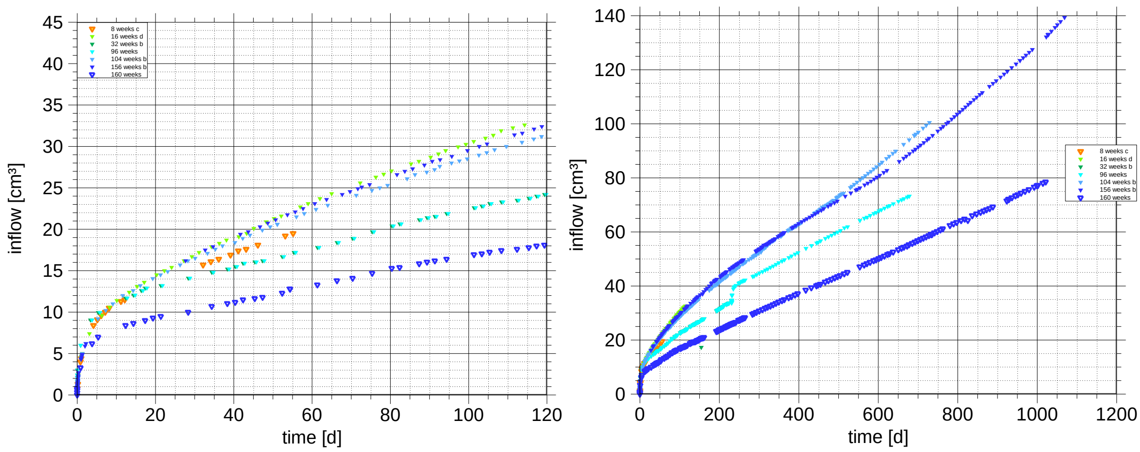


Fig. 4.15 Accumulated water mass for the 7 tests during 120 days (left) and 1200 days (right) (new set-up)

4.2.6 Summary and conclusions

All in all 33 uptake tests with varying running times up to 173 weeks against a high temperature gradient have been performed, 26 test in the originally devised set-up and seven tests in cells that had been strengthened against the swelling pressure exerted by the wetted bentonite samples. The experimental set-up was optimised towards a linear temperature gradient along the cell axis. Repeating all tests up to a running time of 16 weeks showed a good reproducibility of the measurements.

The target of finding out about the steady-state conditions at the end of re-saturation against a temperature gradient was missed, though. It had been expected that water uptake would have come to an end under these conditions, but an end of water uptake was not reached in any of the tests. Instead of converging towards zero, the observed uptake rate became even more or less constant after a few months.

In the longer running tests the amount of water entering the cells was exceeding the capacity of the bentonite for water uptake significantly while the samples proved to be far from fully saturated. This observation indicates leakage from the cells, probably in form of water vapour. Such a leakage could have formed if the swelling pressure had been underestimated while constructing the cells and the rings had been separated.

Two unexpected features were found in the evolution of the water content distribution, firstly the forming of the steep moisture front, and, secondly, the apparently steady growing of the highly saturated zone at the water inlet. The latter is a clear indication of swelling which underpins the idea of a swelling pressure induced leakage.

While the location(s) for such a leakage cannot be determined directly it seems to be likely that it would be rather in the zone of high swelling than in the dried-out zone since friction at the ring walls would be higher in the wet, swollen part. This would explain the steep moisture front because vapour would be drawn from the moisture front towards the leak(s).

Under such conditions the monitoring of the water uptake leads to the conclusion that a dynamic equilibrium between water uptake and water loss via leakage had been reached when the uptake rate became constant. The measured water content profiles would then not be representing the uptake conditions at the time of test termination but at a much earlier and rather difficult to determine point in time. With some effort the obtained water content profiles might at least be related to a certain time span with the help of the water uptake curves. However, since neither locations nor numbers of leaks are known this work would be rather pointless.

Further insight could have been gained by numerical modelling of this experiment. It has to be assumed, though, that the forming of leaks is rather a local phenomenon than an axisymmetric one. Modelling would therefore have required a fully three-dimensional treatment of the problem while the code VIPER which had been foreseen for modelling is not yet far enough developed to do so. Modelling the experiment was therefore abandoned.

The final conclusion from this exercise sounds a bit trivial but is to be taken seriously: the experimental effort to provide conclusive data about the end state of water uptake against a significant thermal gradient is considerable. Unfortunately, the work presented here has just added to several other not successful attempts. The construction of a fully operative test cell thus remains to be a challenge.

4.3 Microbial processes

4.3.1 Clay

Based on the results of preceding studies, which indicated that sulfate reducing bacteria are not active or mobile in a saturated bentonite with a density above 1.5 or 1.9 g/cm^3, a conclusion was made by Nagra in the Entsorgungsnachweis project /NTB 02/ that it is to be expected that bacteria will have a negligible impact on canister corrosion and radionuclide transport in highly compacted bentonite. In a similar Swedish project, SKB suggested that the swelling pressure of at least 2 MPa developing in a saturated bentonite with a density above 2.0 g/cm^3 will prevent any microbial activity /SKB 06/.

Later laboratory and in situ studies revealed however that sulfate reducing bacteria remain active even at the latter density /MAS 10/. Moreover, the size of microbial population shows nearly no decrease as the saturated bentonite density increases from 1.8 to 2.15 g/cm^3 /STR 11/. Survival of microbes, typically being micrometer-sized, in compacted clays, in which only a negligible fraction of pores has such a size, was so far explained by either:

(i) a survival in infrequent larger pores, which are characteristic for the interfaces between clay mineral aggregates and between those and grains of accessory minerals such as quartz /PRI 10/, or
(ii) a transformation into a smaller form, which can reduce the cell volume by up to 60 – 70 % through cell division without an accompanying growth or through a continuous shrinking /KJE 84/, or
(iii) a compensation for the external mechanical pressure by the internal cell pressure, which is currently known to maintain cell growth at external pressures of up to 120 MPa and cell viability up to 800 – 900 MPa /VAN 11/.

A further ability of some bacterial genera, which assists them in surviving under conditions of lacking or insufficient supply of nutrients, is the formation of endospores /NIC 00/. In this state, bacteria are able to survive the temperatures, which are 30 - 40 °C higher than the lethal ones for bacteria in an active state. The survival time of endospores under dry conditions is about 1000 times higher than under moist conditions. Relevantly for a repository in clay, the upper temperature limit for the activity of sulfate- and Fe(III)-reducing bacteria, which are able to form endospores, is about 95 °C and 121 °C, respectively /MEL 11/.

The above discussion allows a formulation of the following requirements to the properties of bentonite buffer, which may effectively minimize the possible effect of microbial activity in a HLW/SF repository:

- The lowest possible content of organic carbon in order to limit the most important nutrient.

- The dry density of the buffer should be high enough in order its saturated density after filling up the voids to exceed 2.0 g/cm^3. A higher density would result in a further reduction of microbial activity. The latter may also be reduced by choosing a bentonite with a higher content of montmorillonite.
- A thermal treatment of bentonite – preferably after the emplacement in the repository – at 125 °C or 150 °C for eliminating endospores of sulfate-reducing bacteria or Fe(III)-reducing bacteria for a few hours or days under moist conditions within buffer or for a few months or years under dry conditions. A lower treatment temperature can be chosen upon increasing the duration of the treatment.

The work aimed at obtaining a quantitative estimation of the maximum possible effect of microbial processes in a final repository for HAW/SF in a clay rock resulted in a conclusion that such estimation does require the application of a dedicated software tool because of the far too complex system of competing or synergistic microbial subpopulations interacting with different repository components. These interactions are not only distributed over the whole repository space but also develop within a timescale of years, possibly proceeding for several thousand years, and are influenced by the evolutions of temperature, pore space and nutrient concentrations within the repository system. To account for these evolutions, the population dynamics of microbial community and its interactions with the repository components within a reasonable working effort, a use of an on-the-shelf software tool would be a preferable option.

A review of the most commonly used widely available reactive transport codes /STE 14/ provides a conceptual description of the implementation of microbial processes, amongst other relevant processes, in these codes. Owing the importance of these processes in many subsurface environments, more sophisticated treatments of microbial community function that are coupled to environmental conditions are considered as possible in the future developments of these codes.

The use of Generalized Repository Model (GRM) in the frame of the LLWR Environmental Safety Case for Drigg Low Level Waste Repository in the United Kingdom represents an example of the application of a reactive transport code with implemented microbial processes in a safety case /SMA 11/. GRM is a reactive-transport program that is capable of modelling the pH and redox conditions associated with the degradation of organic and metal containing wastes and the interactions with engineered barriers and groundwater /GRA 03/. The GRM considers the main aerobic and anaerobic microbial processes of respiration, denitrification, iron and sulfate reduction, fermentation and methanogenesis. The extent of the microbial processes, governed by kinetic data and the availability of reactants (microbial substrates and electron donors and acceptors) determines the redox potential of the system. The model outputs a wide range of chemical and microbiological data and radionuclide concentrations and fluxes in groundwater and gas.

4.3.2 Rock salt

4.3.2.1 Overview of the relevant microbial processes

A bachelor thesis titled “Mikrobielle Prozesse in Salzgesteinen” was prepared by Thekla-Regine Schramm /SCH 15/ in the course of the work on the project. This thesis gives examples of the occurrences of viable or active microorganisms in salt solutions similar to those to be expected in a repository environment in a salt rock. It describes the strategies used by the microorganisms to stay alive at such harsh conditions and their taxonometric classification according to the different salt concentrations necessary for their metabolic activity. The possible sources of energy for a long-term survival are addressed as well. A detailed discussion is then given to the microbial processes of sulfate reduction, methane production and iron(III) reduction, which are of importance for the assessments of long-term performance of a final repository. Finally, taking into account of microbial processes in the performance assessment is exemplified for the Waste Isolation Pilot Plant site in New Mexico (USA).

4.3.2.2 Contribution to NEA natural analogue workshop

An overview of experimental findings and field studies on survival of microbes in ancient rock salt is given /MEL 14/, which suggests that indigenous microbes can survive over geological periods of time in rock salt, see also Chapter 4.4.1.3. Microbes introduced into rock salt from the surface as a result of contamination may remain as well viable there for a considerable time. Microbial species retaining the ability to actively metabolise in saturated brines include those which produce corrosive substances and gases. Therefore, microbial activity may be of relevance for long-term performance of deep geological repositories in rock salt and needs to be evaluated.

Microbes capable of exerting – either negative or positive – impact on the long-term performance of a radioactive waste repository are indigenous to rock salt and – possibly added by microbial species introduced during mining or drilling activities – may be present in abundances comparable to those observed in deep subsurface sediments.

Rock salts can contain electron donors and acceptors in amounts sufficient for microbes to remain active for very long periods of time. Additional sources of electron donors and acceptors will inevitably be added to the repository system as a result of repository excavation and placement of radioactive waste, backfill and sealing materials.

Hence, a microbiological exploration of repository environments in rock salts and an evaluation of the maximum microbial effect in long-term performance assessments for a deep geological repository for high-level radioactive waste and spent nuclear fuel in rock salt appear to be necessary. In case that the microbial effect might be assessed to be negative and significant, an elaboration of possible measures to inhibit or impede microbial activity might be an option for a repository design.

4.3.2.3 Contribution to salt club

GRS has contributed to the report on the microbial processes relevant for nuclear waste repositories in rock salt /SWA 16/ and to the respective presentation by Julie Swanson (Los Alamos National Laboratory - Carlsbad Operations, Carlsbad, NM, USA) presented to the NEA Salt Club.

This report summarizes the potential role of microorganisms in salt-based nuclear waste repositories using available information on the microbial ecology of hypersaline environments, the bioenergetics of survival under high ionic strength conditions, and “repository microbiology” related studies. In order to affect repository performance, microorganisms must be present and, in most cases, active. Subterranean salt settings contain a unique community of microorganisms with limited metabolic capacity. The additional constraints of repository conditions and waste and barrier constituents suggest that the overall effect of such microorganisms may be severely limited in the near-field.

It states that the microbial communities present in hypersaline settings are limited in both structural and functional diversity. This is because, in order to survive at high salt concentrations, these organisms must osmotically balance their internal and external environments. This limits their ability to perform certain modes of metabolism, based on the energy required for survival and the energy derived from a given reaction. At the highest salt concentrations, extremely halophilic Archaea are dominant members of the microbial population because of their ability to balance osmotic pressure using a low-energy strategy. These organisms are almost all aerobic with limited anaerobic and fermentative capability, thus their role in repository microbiology may be confined to early oxic periods. Still, they are able to survive tens of thousands of years encased in salt, such that they will be present throughout repository history. Some extremely halophilic Bacteria also exist in hypersaline environments. In general, these organisms will have a much more diverse metabolic repertoire, including aerobic, anaerobic, and fermentative capabilities. However, these capabilities narrow as salt concentration increases, due to the high-energy cost strategy utilized by bacteria to maintain osmotic balance. Bacteria present in repository waste or introduced during mining operations are not likely to be halophilic and may not survive long-term. However, the role of microorganisms within drums may be significant.

GRS contributions specifically concerned, first of all; a consideration of the probable pressure effect on the vitality and activity of the exogenous microorganisms, on the possible microbial metabolic pathways, and on cellulose degradation at the repository conditions was suggested. Indeed, the experimental evidence, on which the argumentations in the report rely on, applies in the far most cases to the pressures which are at – or not substantially above – the atmospheric one of 0.1 MPa. On the contrary, the pressure at the depth of several hundred meters below ground in a salt formation is as high as ~10 MPa.

In this relation, e. g. the results of the study /MOL 04/ may be referred to, which show that microorganisms, for which a salinity of 4 M NaCl is lethal at the atmospheric pressure, survive at this salinity when the pressure equals 200 MPa. Allowedly, the latter value is much higher than the value of 10 MPa. Still, the latter work did not study the effects of intermediate pressures. The open question was accordingly formulated concerning the effects of the repository in situ pressures on the vitality and activity of the exogenous microorganisms and activity of the indigenous microorganisms found in the salt mines.

Furthermore, the methanogenesis using repository substrates (i. e., H_2 + CO_2 or acetate) is considered thermodynamically infeasible at NaCl concentrations above 120 g/L at the standard conditions (at least with respect to pressure). The open question is then whether it still will be inhibited as the pressure increases in the repository. In the discussion on this particular process, a consideration of the results by /GIL 06/ was referred to, which shows that bioenergetic constraints on metabolizing the available acetate, CO_2, and H_2 under hypersaline conditions possibly led to the slow rate of CH_4 accumulation, relative to CO_2, but not to the complete inhibition of the methanogenesis.

Concerning the activity of cellulose degrading microorganisms in the underground, the observation by /VRE 98/ was argued to be relevant that although virtually all hypersaline lakes contain large amounts of dead plant material, the Salado formation contains no sign of fossilized organics but detectable populations of cellulose-degrading microbes. Therefore, an open question remains concerning providing evidence that the cellulose degrading microorganisms of the Salado formation were active only in the brines and not at its early or advanced development stages.

As the second general issue, it should be taken in consideration that the design of the repository and the disposed radioactive waste determine whether actinides or fission or activation products may be dominating the projected exposure dose. For instance, a preliminary safety assessment for Gorleben has identified an activation product ^{59}Ni and a fission product ^{93}Zr as the dissolved radionuclides dominating the radioactivity fluxes at the border of the containment-providing zone within the Gorleben diapir after one million years /LAR 13/. The same report shows also the high relevance of the gas-phase transport of an activation product ^{14}C – as $^{14}CO_2$ – for the radiological consequences of the modeled repository for irradiated fuel assemblies and their end pieces in the Gorleben diapir.

The latter two occasions in the report by /LAR 13/ show that an assumption about the gas-tightness of the canisters for 500 years, which is the time during which the waste canisters should remain in a condition allowing their recovery as regulated by German law, strongly reduces the predicted gas-phase transport of ^{14}C. Furthermore, without such an assumption, the radiological consequences show a strong dependence on the canister corrosion rate, which governs the time of the ^{14}C release from the canisters. Since microbial processes are known to be able to accelerate the corrosion and be able to switch it into a pitting one, meeting the requirement of the integrity of waste canisters for 500 years will depend on whether the microbial activities will be negligible in that period of time.

In an issue important for the estimation of viability of microorganisms, the results of /WIE 12/ for halites in Atacama Desert show that water condensation in halite strongly depends on the pore size and can occur at as low relative humidity as of ~30 %, and as such considerably below the considered otherwise relative humidity of 75 % and above as a prerequisite for a moist environment in salt.

With respect to oxygen depletion after repository closure, as revealed in in situ experiments in Äspö HRL in Sweden, oxygen in a repository can be used up by microbes within few days /PUI 1/. The possible importance of this process for a repository in salt should be evaluated along with the reference scenario, in which the oxygen depletion is governed by the corrosion of waste canisters in a repository.

4.4 Natural analogues

Because of the complexity and the geological time frame to be considered in a safety case for a deep geological repository, a substantial knowledge of geological, hydrogeological and radiochemical processes is of great importance. From this point of view deep insights into relevant “natural” geological processes may contribute substantially to system understanding and finally to the compilation of the safety case. As in other countries, a compliance period of 1 million years is required in Germany. Such a long time span makes it difficult for predictive modelling to fully overcome the remaining uncertainties that accompany "short"-term lab experiments and field studies. This is particularly true for the geological phase, where geochemical and hydrogeological processes in particular are relevant for fulfilling the safety functions. However, the comparison of such results with processes in nature, which show a reasonable similarity, may help in gaining greater confidence in those data as well as in the numerical models based on them. The respective natural, anthropogenic, archaeological or industrial systems which have some definable similarity with a radioactive waste repository and its surrounding environment, are usually denoted as natural analogues /MIL 06/. In its basic form, a natural analogue study can be any type of investigation of any relevant natural system, as long as it provides quantitative or qualitative information which can be used to support (and build confidence in) geological disposal /ALE 15/.

The main value of natural analogue studies is to provide information about a geological system (evolution), i. e. the characteristics of processes occurring over very long time scales. In general, the direct use of quantitative information from natural analogue studies in a safety case has been mostly limited, because it is very difficult to extract hard numerical data from complex natural systems, where initial and boundary conditions cannot be fully defined. Indirectly this information could, however, be very valuable in a supportive sense. Therefore, natural analogues are an integral component of the safety case in national repository programmes /ALE 15/, /NAG 02/, /MIL 02/, /SMA 06/, /PUU 10/, /LOP 04/. Moreover, the regulatory authorities explicitly require safety assessments to be supported by qualitative arguments for a system's long-term safety /NEA 13/.

During the project major work on analogues has been devoted to

- analogues for safety cases in rock salt, particularly for organization and evaluation of a workshop in the frame of NEA's salt club,
- a wrap-up of the natural analogue study at Ruprechtov with compilation of the lessons learnt, and
- the compilation of natural analogue studies for a repository in clay rock and evaluation how they are related to the FEP and contribute to the safety goals.

4.4.1 Analogues for safety cases in rock salt

Rock salt is a potential host rock for a geological repository for the disposal of high-level and long-lived wastes because of its favourable characteristics. Due to its very low hydraulic conductivity and its ability to deform plastically under stress, rock salt can, in the right circumstances, provide robust, long-term isolation of the waste from groundwater.

Best practice in repository safety cases is based on the use of multiple lines of reasoning /NEA 12/, and one important line of reasoning for improving repository system understanding is the use of natural analogues.

From 4th to 6th September 2012 the Project Management Agency Karlsruhe – Water Technology and Waste Management (PTKA-WTE) and the Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH hosted in the frame of the Salt Club activities (see Chapter 3.4) a joint workshop on “Natural Analogues for Safety Cases of Repositories in Rock Salt”. The workshop took place in Braunschweig, Germany. The objective of the workshop was to compile studies about natural as well as anthropogenic analogues (NA) from different countries to be potentially used within safety cases for radioactive waste repositories in salt formations.

The workshop was structured around the following topics:

- general aspects of analogues,
- status of disposal programmes in the Salt Club member states,
- integrity of rock salt,
- integrity of technical barriers,
- microbial, chemical and transport processes.

In the second part of the workshop four parallel working sessions discussed the status of NA in salt, the key unresolved issues, high priority recommendations for future NA studies for salt and possible recommendations to the Salt Club. The results of the discussion are summarised below.

The workshop attracted both organizations working actively in the field of NA, and also other organizations, e. g. regulatory bodies that wished to be informed on the status and practical applicability of NA, as well as companies from the salt mining and the oil/gas storage industry that presented their practical experiences.

A detailed description including the presentations of the workshop are contained in the Workshop Proceedings /NEA 14/. The summary with the observations and some recommendations drawn from the presentations and discussions at the workshop is also listed in the following chapters. For the sake of convenience, the term ‘natural analogue’ is used here in its widest sense and includes anthropogenic analogues where appropriate.

4.4.1.1 General aspects of natural analogues for the safety case

There has been considerable development in thinking with regards to natural analogues over the last decades. Early analogue studies were very often simply geochemical research projects intended to provide field data concerning the processes (and their rates, where possible) that control radionuclide migration, e. g. in and around uranium orebodies. These studies were often planned and interpreted with limited involvement from experts in safety cases.

More recently, there has been a recognition that natural analogues can positively contribute to multiple lines of reasoning in a safety case, along with other forms of study such as paleo-hydrogeology and the use of complementary safety indicators /NEA 12/. It is now widely accepted that there are multiple ways in which natural analogues can support a modern safety case for geological disposal /MIL 06/. For example, as part of the assessment basis they can be useful for

- features, events and processes (FEP) identification and screening, and scenario development,
- conceptual model development,
- data provision,
- uncertainty management,
- numerical model, code and data testing and confidence building, and finally
- in a broader sense, confidence building of experts and laypersons.

More generally, natural analogues may be useful for helping compile the evidence, analyses and arguments and to place the safety case and its results into context. Lastly, there is the possibility that analogues may be useful during communication and dialogue with stakeholders, provided the analogues are meaningful to the audience and appropriately used.

It should be noted that there is a distinction between the identification of a potential study or site, and it being accepted as a relevant analogue to support a safety case. Potential analogues (and analogue-derived information) need to be critically evaluated to ensure their appropriateness to both the disposal concept and safety strategy, as well as to the safety assessment methodology.

Sometimes in the early days of natural analogue studies, interesting geological and geochemical systems were first identified and then attempts were made to compare them (back-fit them) to the repository system and the safety case. There was sometimes a lack of rigour when choosing analogues and when applying ‘quality assurance’ checks to the information derived from analogue studies. This led to some cases of misrepresentation of the equivalence between natural and repository systems, and overinterpretation of analogue information. In a reversal of this approach, *Alexander, McKinley & Kawamura* suggested in future a ‘top-down’ method should be followed to identifying natural analogues. In this, goals for natural analogues are first set (such as the goal to demonstrate stability of the host rock) and then appropriate analogue sites are sought or relevant analogue information extracted from the published literature. This goal-setting approach for analogues has some parallels to the recent development of defining safety functions for the disposal system and its components. Setting goals for natural analogue studies may be one way (alongside laboratory and modelling studies) to seek information to help confirm that a safety function is met.

As previously mentioned, many different natural systems and sites, from a number of countries, were discussed at the workshop. Several of these have not previously been recognised or examined as potential analogues. The broad range of examples presented illustrates that the scope of analogues for rock salt is potentially extensive. Without diluting the overarching concept of natural analogues, it may sometimes be useful to recognise the different 'types' of analogues, for example:

- industrial analogues - such as gas storage caverns in rock salt that may provide information on aspects to do with the geo-mechanical behaviour of the rock during excavation of the repository and of technical barriers;
- contemporary analogues - that may provide information on short-term processes, such as the response of the rock mass during reestablishment of THMC equilibria;
- operational analogues - that provide information on practical aspects of constructing and closing excavations in salt, which are likely to be increasingly useful as programmes move towards implementation;
- national analogues - that place the repository into a national or regional context by providing local examples that may be most meaningful to the public and other stakeholders;
- social analogues - that may refer to aspects of demographics and the behaviours, e. g. in decision making, of the current generation that may be analogous to future populations;
- negative or anti analogues - that highlight that processes and rates can be more aggressive and faster in certain environments than is often assumed for repository conditions i. e. most archaeological evidence suggests iron artefacts corrode away, and are not preserved;
- self analogues - which refers to information derived from the actual repository site, rather than another location.

An important aspect that was stressed from the discussion at the workshop of the possible 'types' of analogue studies is the importance of correct and unambiguous terminology to avoid possible misunderstandings between different audiences. This is an issue for the safety case as a whole because it should be recognised that the meaning of certain words used by the public in common speech is sometimes different to the usage by experts (the word 'risk' for example), and even occasionally between different groups of experts.

In particular, there can be differences of opinion in what represents an appropriate analogue site or system, and what does not. The question of 'equivalence' with a repository system is fundamental to the concept of natural analogues. It is clear that if analogue information is used in safety assessment modelling, it should be of the highest quality and also that the similarities and differences between the analogue and repository systems should be understood and transparently described.

Decision making throughout a repository development programme is iterative, and different but appropriate levels of information are required at each key stage and decision point. It follows that qualitative analogue information and semi-qualitative analogue data may be used in the early stages of a programme to help underpin certain preliminary decisions. For example, the weight of archaeological evidence on metal corrosion may be used (when combined with laboratory data) to narrow down the choice of potential container materials. At later stages in the repository development programme, however, such qualitative analogue information would be insufficient to support detailed optioneering or design optimisation work, and more quantitative information would be needed.

As suggested by *Pescatore*, one approach to reflect these different applications of analogues within a repository development programme may be to adopt a hierarchy of concepts that could be represented by using alternative terms (with slightly different definitions) such as 'anecdotes', 'analogies' and 'analogues' to indicate increasing levels of similarity between the natural and repository systems. This is a novel suggestion and one that might be worthy of further consideration. It is worth noting that this suggestion is born partly out of work by the OECD/NEA Forum for Stakeholder Confidence (FSC) that highlighted the importance of terminology for confidence building.

There has long been a debate regarding the potential value of using analogues for public communication and confidence building. The visual appeal and everyday context of some analogues (e. g. the longevity of Roman buildings still standing in many European cities) have often been cited as reasons why analogues could be useful when engaging in dialogue with non-technical audiences. Several national programmes have used analogues in this way in the early days of analogue studies (e. g. Spain, Sweden and UK) but, despite this, there is no solid evidence to suggest that they have proved useful for explaining disposal concepts and long-term safety. Part of the nervousness for using analogues for public communication may be related to the concern of 'overinterpretation' but provided that analogues are used appropriately there seems to be no reason why qualitative analogues should not be used for general confidence building as a parallel activity to using quantitative analogues for technical input to safety assessment.

Given the points raised during discussion at the workshop, it is evident that there are a number of issues that could usefully be addressed in the future. These include:

- Care should be taken to identify the various roles that natural analogues could play within the overall safety case, understanding that different applications are possible and that each may have their own specific requirements.

- Within the context of safety assessment, analogue studies and analogue information should be critically assessed, with particular attention paid to understanding the implications of the differences between the analogue and repository systems (such as the boundary conditions), as well as the similarities. Natural analogues should not be considered in isolation. Their value is enhanced when used in combination with other multiple lines of reasoning, such as paleo-hydrogeological investigations, when the advantages of one can be used to balance the drawbacks of another.

- Care should always be taken to avoid overinterpretation and abuse of analogue information. In the context of preliminary decision making and for concept development, the requirements for analogues may be more relaxed than for detailed safety assessment modelling.

- The use of analogues for public communication and dialogue remains unproven and is an area worthy of further consideration. It is likely that analogues with a familiar and local context may be most useful in this regard.

4.4.1.2 The application of analogues in national repository development programmes based on rock salt

The various national repository development programmes around the world investigating disposal in rock salt are advancing at different rates. This is due, in part, to variations in government policy but also the practicalities of identifying suitable geological environments, host communities and progressing the underpinning technical work. Advanced programmes are the WIPP site (New Mexico, USA) and Morsleben (Saxony-Anhalt, Germany). These disposal sites vary, however, in so far as WIPP remains operational but Morsleben is to be decommissioned. A number of other national programmes have identified rock salt as a preferred host rock but have not yet chosen a candidate site (e. g. Poland), and others retain rock salt alongside crystalline and argillaceous rocks as a possible host rock type in an open siting process (e. g. the UK, The Netherlands, Belarus).

The use of natural analogues in disposal programmes based on rock salt to date is also variable. As one example natural analogues were undertaken in support of WIPP to aid system understanding but did not feature directly in the formal safety case for the facility /NEA 00/. The types of analogue studies that were performed include /MIL 93/:

- uranium migration studies in the fractured Culebra Dolomite aquifer that overlies the bedded salt deposits that host the repository;
- earthquake activity and seismic impacts (rock bursts in salt mines); and
- material corrosion rate assessments based on preservation of artefacts found in old salt mines.

Although natural analogues did feature within the WIPP project, in general, fewer analogues studies have been undertaken in rock salt /NOS 08b/, /BRA 14/ than in other rock types, such as in crystalline rocks, e. g. /MIL 06/, /LAV 08/. The reason for this is not entirely obvious, but probably simply relates to the fact that the national programmes that initially developed the concept of analogues in the 1980s (at least in Europe, notably Switzerland, Sweden and UK) were not focussed on rock salt.

Germany started investigations into NA in the mid-nineties after a national workshop considering this topic was organized. This workshop discussed some R&D projects that had been conducted, as well as some natural analogues that had already been running for several years such as the Ruprechtov NA in the Czech Republic (see, e. g.

/NOS 08a/, /NOS 09/ and Chapter 4.4.3). After the workshop, a comprehensive study on the use of NA was undertaken /NOS 08b/, /BRA 14/ and presented.

Important outcomes of that workshop were the conclusion to proceed systematically in the use of NA, and the identification of many different natural systems and sites, from different countries, which expands the portfolio of analogue studies that are potentially relevant to safety cases for disposal in rock salt.

Looking to the future, there is likely to be greater interest and use of analogues within disposal programmes based on rock salt following the Salt Club initiative. As an example, *Wolf, Noseck and Steininger* explained how Germany is preparing for a new strategy that intends to use natural analogues as an integral component in its safety case methodology. As an early part of the process, a comprehensive compilation and assessment of natural analogues relevant to rock salt is underway. An interesting and unique aspect of this work is an attempt to categorise analogue studies in a structured manner according to their relevance to the important elements of the German safety and assessment concept: (1) the integrity of the geological barrier, (2) the integrity of the geotechnical barriers, and (3) radionuclide release scenarios. The availability and quality of study reports is also assessed to identify which analogues are sufficiently well documented to be of possible value for either technical confidence building or public confidence building.

The WIPP and Morsleben repositories provide an opportunity for learning based on experience from construction and operation of these facilities. This is a form of 'implementation analogue' albeit more applicable to practical operations than development of the safety case. Various lessons learned from the WIPP operating experience that could be applicable to other repositories include such things as to avoid mixing different wastes in the same vault, and to adopt a flexible programme of cavern excavation and waste emplacement, to mitigate against delays in waste shipments etc.

Finally, a particular feature of rock salt is that formations can, in some cases, be laterally extensive and internally homogenous. In Europe, certain formations extend across national boundaries, such as the Zechstein which extends from across northern Europe from the UK to Poland. This provides an opportunity for increased international cooperation and research into analogue studies related to disposal in rock salt.

4.4.1.3 Rock salt specific analogue results

The primary characteristics (and safety functions) of rock salt that contribute to long-term isolation of the waste from the accessible environment are (1) very low hydraulic conductivity, and (2) the ability to deform plastically under stress, so discontinuities, which might present potential pathways, can 'self seal'. These are somewhat different to the characteristics of other potential host rocks that provide isolation by processes such as radionuclide sorption, dilution and dispersion along groundwater flow paths. As a consequence, natural analogue studies relevant to rock salt are very often focussed on containment processes rather than transport/retardation processes.

Most analogues studies performed so far on rock salt have investigated processes that may impact on the integrity of the salt and cause a reduction in its containment performance. These studies seek to improve conceptual understanding of relevant THMC process mechanisms, couplings and boundary conditions, as well as to quantify their rates and limits. A number of studies were presented and discussed at the workshop, and some highlights from these are given below.

- Thermal processes have been investigated around volcanic dyke and sill intrusions into rock salt. These may be analogous to the heat generated by vitrified HLW and spent fuels, although the temperatures in a repository near-field (a likely maximum of c. 100 – 200 °C depending on the repository design) will be much lower than experienced in a contact metamorphic situation (c. 1 000 °C). As explained by *Rempe*, natural analogues thus provide practical examples of worst case scenarios in which the containment performance of rock salt would not be compromised.

  Hydraulic processes have been investigated in several analogue systems. Observations and measurements of water inflows in Polish salt mines presented by *Dulinski* illustrate the potential use of isotopes to characterize the age and origin of brines in salt formations, see Fig. 4.16. On that basis syngenetic (intrasalinar) water appearances can be clearly distinguished from recent (Quaternary) and modern waters. Such measurements are important to identify the source of waters not only in salt mines, which have been excavated for several tens to hundreds of years, but also in salt repositories where water intrusion from the adjacent geologic formations can impact the safe operation of the mine and have to be investigated. *Urai* illustrated that free water can be present in rock salt on spatial scales ranging from micrometre sized fluid inclusions to tens of metres sized brine pockets. A key observation of this work is that fluid inclusions may be separate and immobile under normal conditions but can become mobile if the stress conditions change. Accumulations of brine in larger pockets can also rise upwards through salt deposits, driven by buoyancy. Similarly, oil from big intrasalinar carbonatic rock inclusions has been observed to migrate through deformed and intensively uprising salt over large distances, as observed in oil deposits in Oman. This salt dome is characterized by a high content of hydrocarbons and is in the very active diapiric phase. However, this behaviour cannot be observed in the salt domes of the Northern German Zechstein Basin in the post diapiric phase. The brine pockets around the WIPP facility are also observed to be immobile due to the static geological conditions.

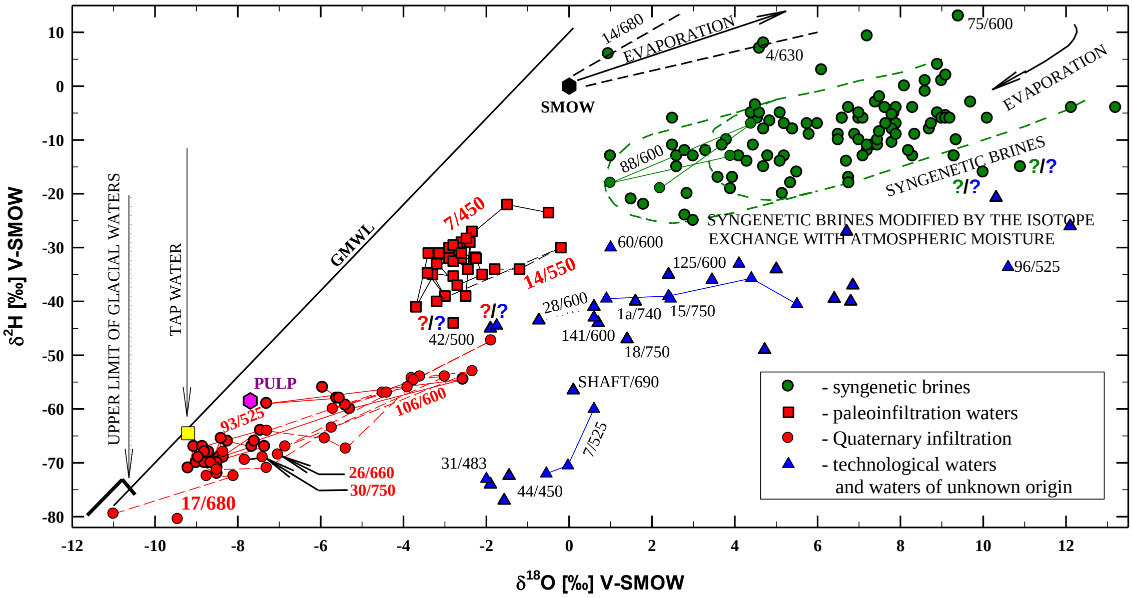


Fig. 4.16 Stable isotope composition of waters occurring in the Kłodawa Salt Mine with different origin (selected data, /DUL 13/)

- Mechanical processes in rock salt have been investigated at numerous sites and on different spatial scales. On a large scale, 3D seismic modelling of salt domes by the oil and gas industry, and described by *Urai*, show the influence of the anhydrite layers that are mechanically stronger than the associated halite in the salt dome structure. This is supported by laboratory studies, such as those described by *Mertineit, Hammer, Zulauf, Zulauf and Schulze*, that show when subject to stress, halite will deform by plastic flow but anhydrite will deform by brittle fracture. Because of the creeping of rock salt the fractures healed, and consequently the permeability of the rock remains very low /HAM 12/. In a repository environment, the safety case must show that these fractures are not possible pathways for groundwater flow. Detailed observations from exposures and boreholes at the Gorleben salt dome and Morsleben repository presented by *Hammer, Behlau, Mingerzahn and Mertineit* showed, however, that the anhydrite at Gorleben and Morsleben (Hauptanhydrite, z3HA, Gorleben-Bank, z3OSM and Anhydritmittelsalz, z3AM) do not contain large-scale interconnected porosity, but clear evidence of secondary sealing in the fractures, see Fig. 4.17. This is a good example of how laboratory, field and analogue studies can be combined to increase process understanding and, in particular, the issue of spatial scaling.

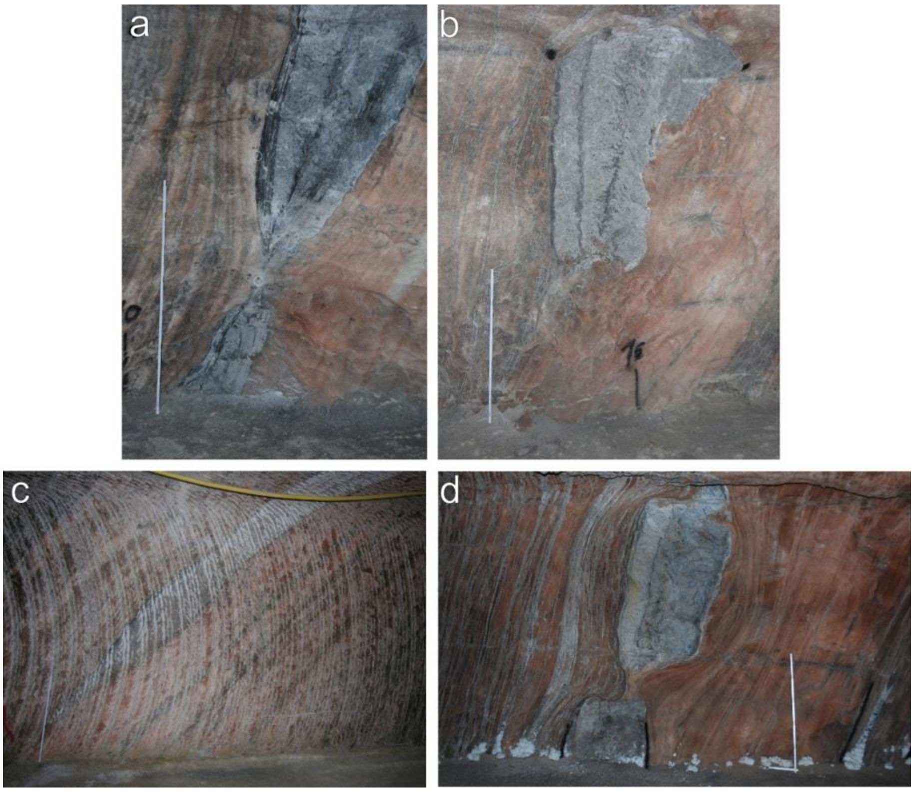


Fig. 4.17 Different Boudinage forms in the Anhydritmittelsalz, ERA Morsleben /HAM 12/

- Microbial populations have been recorded in rock salt, including in mines and in brine inclusions, as described by *Meleshyn*, see Fig. 4.18. It is probable, therefore, that microbes will be present in the near-field of a repository, but it is unclear if they will be viable in the post-closure environment and affect repository performance (e. g. by the production of gas and corrosive substances) and, consequently, whether they need to be explicitly considered in the safety case. Laboratory and field studies (e. g. at WIPP) confirm the presence of ancient indigenous microbes as well as modern introduced species but, to date, few analogue studies have provided convincing data on their viability under repository post-closure conditions.

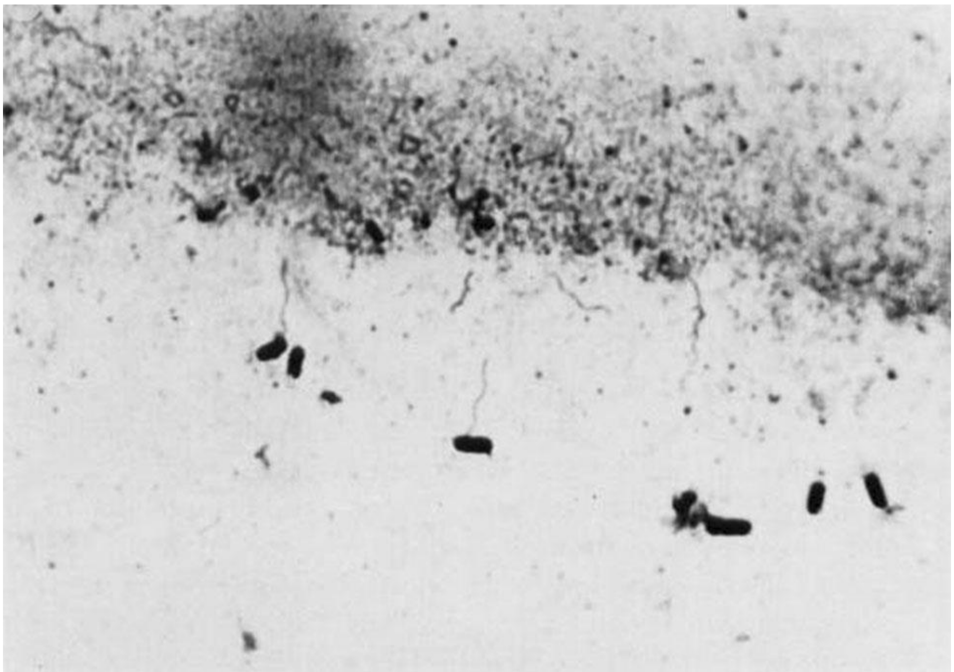


Fig. 4.18 Microbes in the Precambrian salt /MEL 14/ (Source /DOM 63/)

- Certain chemical processes that may affect the safety performance of a repository might potentially be more significant in rock salt than in other geological environments. Of particular interest are the possible consequences of reactions involving hydrocarbons because of the common geological association between oil and gas deposits, and salt domes. Hydrocarbons can be dispersed throughout salt and readily detected in mines, such as at Gorleben, as illustrated by *Bracke*. During repository operations, accumulation of flammable gas may increase the risk of explosion. It must be dealt with in the construction and operational safety assessments for the disposal facility. In the post-closure period, thermochemical reduction of sulphates by hydrocarbons has been postulated as a mechanism that may lead to production of water and corrosive substances that could lead to a loss of integrity of the rock salt. As with microbial processes, however, few analogue studies have provided information on the likelihood and consequences of this processes occurring under repository conditions.

  Releases of Ra-226 often dominate the calculated post-closure doses in repository safety assessments due to the assumption of high mobility and the corresponding choice of conservative values for solubility and retardation factors in transport models. Nonetheless, as explained by *Metz, Rosenberg, Böttle and Ganor*, there is analogue evidence to show that Ra can often be retarded by co-precipitation with Ba within $(Ba,Ra)SO_4$ (barite) solid solutions in crystalline and argillaceous environments. More recent studies now indicate that Ra can also be retarded by co-precipitation in saline systems, such as the Ketziot desalination plant in Israel, see Fig. 4.19. These findings are generally supported by appropriate laboratory experiments. However, differences in partition coefficients measured in co-precipitation and re-precipitation experiments, respectively, need to be resolved in further studies, to determine the extent to which the radiobarite co- and re-precipitation systems approach near-equilibrium conditions. Other studies would be useful to extend these observations to systems that more closely resemble the repository environment to determine whether co-precipitation could be taken into account in the safety case for a repository in rock salt to reduce the conservatism in the transport models.

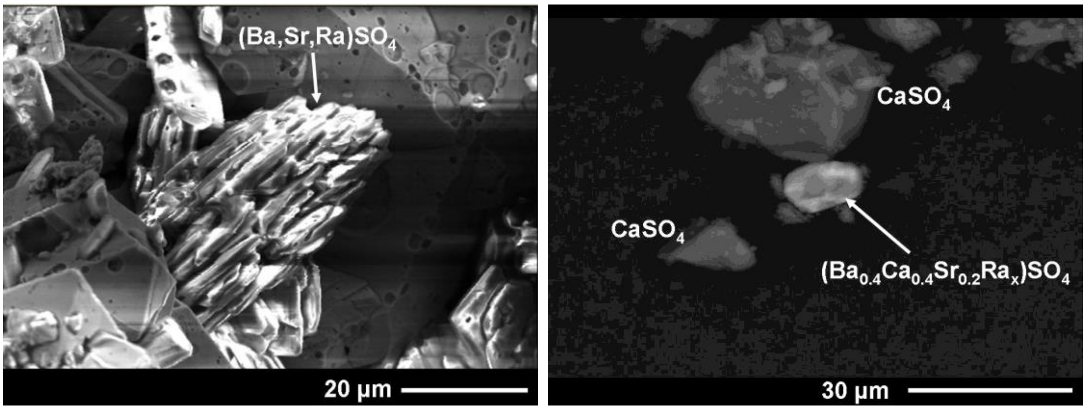


Fig. 4.19 SEM images of ternary and quaternary Ra-bearing barite solid solutions (Metz et al. 2013). Left image (Ba,Sr,Ra)SO_4(s) crystal in a precipitate sampled from a geothermal energy plant in Southern Germany; right image (Ba,Ca,Sr,Ra)SO_4(s) crystal precipitated in pond #1 of the Ketziot desalination facility, Southern Israel (Metz et al. 2013)

It is also clear that the coupling of THMC processes in rock salt is complex, with multiple potential mechanisms that could affect the integrity of rock salt as a geological barrier. Nonetheless, there is also strong evidence from natural systems to confirm that rock salt is a stable environment, and so may provide long-term containment for radioactive wastes, provided that certain boundary conditions are not exceeded. It is clearly important to define the thresholds between a stable and a dynamic situation, and to understand what FEPs may cause a change to occur. These may potentially be internal to the repository system (e. g. a build-up in gas pressure due to corrosion or microbial action) or external (e. g. a change to groundwater flow rates and chemistry driven by climate evolution).

Many processes occurring in rock salt do so over a range of spatial and temporal scales. Notably, fluid migration can occur on the microscopic (grain boundary) to macroscopic (brine pocket) scales. It is important to understand how analogue and laboratory observations could be scaled to the repository environment and assessment time periods, recognising that scaling relationships are unlikely to be linear.

Natural analogue studies alone cannot answer these questions, but they may provide strong collaborative evidence, together with laboratory and modelling studies. When seeking new analogue studies and sites, and when evaluating analogue information, those that have specific relevance to the safety functions and characteristics of rock salt would be most appropriate to consider, recognising that these are different to other rock types, and so may require unique analogues. In particular, analogues that provide information on the low hydraulic conductivity and self-sealing properties of rock salt would be particularly appropriate. In addition, analogues that shine light on the dynamic processes relevant to evolution scenarios for the repository near-field are particularly valuable, most notably those that might provide information on scenarios that could trigger groundwater movement over a large scale.

The studies presented and discussed during the workshop have proven particularly useful for improving the qualitative understanding of processes that occur in rock salt. This is valuable for the safety case and helps build confidence in the conceptual models that underpin the numerical models. The greater challenge for analogue studies is to provide quantitative information that might help set conservatively realistic limits to specific parameter values used in the numerical models, or to help define the thresholds (limits) to environmental conditions that if exceeded cause a change to more dynamic behaviour.

With this in mind, analogues for rock salt should be drawn from a wide range of relevant situations, including modern industrial examples as well as from geological systems, as discussed below.

4.4.1.4 Learning lessons from other industries

Observations from the analogue studies described above give confidence that rock salt can provide long-term containment for radioactive wastes, provided that certain boundary conditions such as temperature, stress, strain, pressure are not exceeded. In addition to the geological barrier, geotechnical barriers like plugs and seals play an important role in the safety concept for repositories in rock salt. The sealing design for the German safety concept is based on backfilling of the open void volumes in the emplacement areas after disposal of the waste with crushed salt. The cross drifts of the disposal areas will be sealed with seals against the main drifts and the transport drifts with seals against the infrastructure area. Shaft seals are needed to prevent water inflow through the shafts. Since credit for these seals is taken for several thousand years in the safety case, analogues information could provide strong arguments for the integrity of such barriers over longer time scales than addressed in laboratory experiments.

An understanding of the nature of the boundary conditions and thresholds mentioned above comes from experience from other large-scale excavations in salt, such as mines and gas storage caverns, as described by *Knauth and Minkley* and also by *Crotogino*. These industrial analogues confirm that rock salt is impermeable to groundwater and gas flow, provided the salt remains undisturbed. Good examples are gas releases induced by blasting or drilling, which are frequent in the Werra potash district /MIN 14/. An exploration hole in the potash mine Unterbreizbach caused the biggest CO_2 gas blow-out (27. to 30. August 2003), and, due to the cooling of the highly pressurised gas, a 5 to 6 m wide and up to 3 m high CO_2 glacier (Fig. 4.20). This geological analogue from potash mining clearly demonstrates the isolation potential of rock salt for millions of years, even for trapped gases under high pressure.

Fig. 4.20 CO_2 glacier after an underground gas breakout in salt rocks /MIN 14/

There are, however, numerous examples where changes to boundary conditions have caused a loss of integrity, leading to collapse of excavations, damage to surface structures and groundwater to flow into tunnels etc. Modelling studies show that this situation may arise if either the minimum stress or dilatancy criteria are exceeded.

Experiences from disposing of hazardous wastes in salt and potash mines were described by *Lukas*. These industrial analogues provide very useful practical information on aspects such as the design of tunnel backfills, plugs and seals. There are now a number of hazardous waste disposal cells, and associated access shafts, that have been closed and sealed (using bentonite and gravel seals keyed into the salt), and these may provide unique opportunities for performance confirmation monitoring of the seals over several decades into the future, and to help in the design of the seals and plugs for a radioactive waste repository. Although clearly very informative, the transferability of industrial analogue information to the repository system needs to be carefully assessed. As is the case with all forms of analogues, the similarities between the conditions of industrial analogues are used for and the repository conditions need to be identified and evaluated, as well as the differences.

For example, there may be different views regarding the stability of excavations in rock salt, and its integrity as a barrier, due to the very different timescales over which it needs to be assessed for disposal compared to other situations. As a consequence, it cannot be assumed that practices (e. g. modelling approaches and facility designs) adopted in one industrial situation can be directly applied to the repository. They can, however, provide a very useful starting point, and one that may avoid duplicating effort. That means, where there is overlap and areas of common interest between radioactive waste disposal and other industries, there may be clear benefits to be gained from cross-industry liaison and collaborative research and exchange of knowledge and experience. This will help to improve conceptual and numerical models for rock salt behaviour and assess its integrity as a barrier over the long-term.

4.4.1.5 Final comments and conclusions

This workshop within the scope of the NEA’s Salt Club represents a rare attempt to identify and evaluate natural analogues specific to disposal concepts in rock salt. The significant differences between the characteristics and safety functions of rock salt compared to other potential host rocks means that there is considerable benefit to this focus. In particular, it is important that analogues for rock salt are found that are relevant to containment processes rather than just transport processes, which has usually been the case for analogues for crystalline and argillaceous host rocks.

Rock salt can be a dynamic environment, with coupled THMC processes occurring that may affect the long-term safety performance of a repository. Natural analogues can, therefore, be equally important for aiding FEP screening and scenario development in the early stages of a safety case, as they are for supporting the subsequent safety assessment modelling calculations.

It is important to realise, however, that there is a difference between observing a process in an analogue system and concluding that the same process will occur and be significant in the repository system. There are many cases where processes seen in nature may be only of secondary importance to the safety of the repository. There are yet others where the potential significance of processes remains an open question. Examples discussed at the workshop include microbial populations and hydrocarbon accumulations; the importance of both for a repository in rock salt is open to debate.

For this reason, analogues need to be fully integrated with the safety assessment modelling strategy. It will often be the case that a natural analogue study will demonstrate that a process may occur under repository conditions but that a mechanistic model may be required to determine its significance.

In the early stages, when a programme may be seeking to identify disposal concepts and reference designs and materials, qualitative information may be sufficient. As the programme proceeds towards design optimisation and formal safety assessments, then there will be an increasing need for more quantitative information.

This raises the concept of ‘fit for purpose’ analogue information. Whilst quality assured work should always be an aim, this is different to treating every analogue study as an academic research project. The objectives of an analogue study should be clearly defined and related to information needs. These needs may vary depending on the status of the repository development programme, and reflect that decision making throughout the programme will be iterative and become progressively more detailed over time

It follows that there is a challenge to all natural analogue studies to progress beyond simple qualitative observation to aid conceptual understanding, and aim to deliver more quantitative results that might help set the parameter values used in the numerical models, or to define the boundary conditions for system behaviour.

For this to be achieved, it will be essential that

- future analogues are based on high-quality science,
- the similarities and differences between an analogue system and the repository system are critically assessed,
- these similarities and differences are clearly explained when the analogue study is described and interpreted, and
- all analogue information used to support the safety case should be properly justified.

Natural analogues for rock salt should not, however, be considered in isolation but are best treated in the safety case in combination with other multiple lines of reasoning, such as paleo-hydrogeology and complementary safety indicators. The reason for this is that no single line of argument can be conclusive, but by combining different arguments, the benefits of one may offset the disadvantages of another.

When seeking new analogue studies and sites, it is particularly useful to have a broad view, and to seek also analogues from modern industrial systems (such as gas storage, mines and oil/gas exploration) as well as from the more traditional natural geological systems. In particular, industrial analogues may provide information e. g. on the response of rock salt to hydromechanical perturbations and help to define the mechanisms that can cause rock salt to stop behaving as a static material and begin to act in a dynamic manner, and may be used also to quantify the threshold at which that change happens. Industrial analogues (e. g. experience from ongoing hazardous waste disposal operations) may also be useful for addressing a number of practical issues such as backfilling, closure and sealing of a repository, and methods for waste retrieval should that be necessary.

There is clear benefit to be gained from exchange of knowledge between scientists/experts and industries involved in rock salt. A number of issues may be of common interest, such as the need to model the behaviour of rock salt and assess its integrity as a barrier.

Despite several decades of analogue study, the value of natural analogues for public communication and dialogue remains unproven. Given that analogues are widely accepted as a significant contributor to the safety case, and that a primary role of the safety case is to build confidence, it is somewhat surprising that no national or international agency has yet undertaken any serious attempt to test analogues as a communication tool with non-technical audiences. Intuition suggests that appropriately chosen analogues that provide meaningful context (e. g. regarding site, materials and timescales) would be useful to help present the safety case to a range of stakeholders.

4.4.1.6 Recommendations for further work

In this section, some recommendations for further activities regarding natural analogue studies relevant to rock salt are provided, on the basis of the discussions and comments made at the workshop. This is not intended to be a comprehensive list of all necessary future work but, rather, to provide some signposts to activities that may bring early benefit to workers in the field.

It is first recommended that all organisations with an interest in analogue studies undertake a systematic review of their key information needs (a gap analysis), and then decide which of these gaps may best be fulfilled by analogue information. In this context, the ‘needs’ are likely to be varied and depend on the stage of the repository development programme and so the required ‘information’ may take different forms, including both hard, numerical data and soft, qualitative observation. The point is clearly to determine the objectives and success criteria for future analogue studies so that they can be better planned.

At an international level, a good starting point for this gap analysis is the Salt Club’s planned FEP Report. It is recommended that this report goes beyond simply describing FEPs but also makes an attempt to identify where analogue information (and other sources of data) exist to support both conceptual understanding and numerical parameterisation of each individual FEP. If no analogue information can be identified, or the existing information is inadequate, then this may suggest an opportunity for a new study. However, it is not credible to suggest that an analogue is needed or available for every FEP.

The early engagement with other industries demonstrated at the workshop is commended, and steps should be made to collaborate or at least exchange information on future studies when there is a common interest. A first priority could be to identify and understand why there are differences in how the integrity of rock salt is perceived and assessed by different industries, and also by their regulatory bodies (e. g. between those regulating nuclear safety and mining operations). Engagement with other industries will also help to identify sources of existing analogue information and potential future analogue studies.

When planning new analogue studies, or when evaluating existing analogue information, there needs to be full integration with safety assessors. This is an old message but one worth repeating. It is important that analogue information is fit for purpose when applied in the safety case to ensure best value can be obtained from the studies.

Similarly, natural analogue studies should be integrated with other parallel geoscientific and observational studies (such as paleo-hydrogeology, natural safety indicators, site characterisation etc.). There should be synergy between the multiple lines of reasoning used in the safety case so that they mutually support each other, rather than being viewed as separate and unrelated activities. The international agencies may take a lead in this area, by ensuring effective dialogue and information sharing between the ongoing initiatives such as the NEA's Salt Club.

Multiple lines of reasoning are intended to help build confidence amongst all stakeholders, including non-technical audiences. In this context, it is recommended that a rigorous attempt is made to evaluate the true potential of analogues for public communication and dialogue through some structured opinion survey. This is an oft debated issue, and there are opposing views as to whether or not analogues help build confidence with non-technical audiences or whether they are a distraction. The work by the NEA's FSC in 2008 began to examine this issue but involved only disposal agencies, rather than the wider stakeholder community. It would be useful to the safety case community as a whole to have some guidance on this issue. The NEA may be best placed to undertake this work.

In addition to the general recommendations above, it was evident from discussions at the workshop that there are some specific technical issues that may benefit from further analogue study, and some of these are listed below. The individual papers provided more details on these and other issues. This is not intended to be a 'shopping list' for funding agencies but a starting point to identify some significant issues and processes in rock salt where analogue information might reasonably be expected to provide further insight, understanding and quantification:

- Compaction of crushed salt backfill and stability of plugs and seals: the backfill and closure components in a repository need to withstand the slow plastic flow and deformation within rock salt. There are several hundreds of years of experience from salt mine operations and closure that might potentially be useful to the design and assessment of the closure components. Recent sealing of shafts at hazardous waste disposal sites in rock salt provide opportunities for performance confirmation monitoring of a closed facility.

- Deformation and blocking of anhydrite: Detailed observations from exposures and boreholes at the Gorleben salt dome and Morsleben repository showed that following deformation the blocks of former anhydrite layers contain no large-scale interconnected porosity, but clear evidence of healing the fractures. Laboratory, field and analogue studies can be combined to increase process understanding and, in particular, the issue of spatial scaling. Examples from other salt domes would provide strong arguments for a safety case underpinning that this process is likely to occur.

- Isotope analyses: Analyses of stable and radiogenic isotopes are of high value to investigate the long-term integrity of salt formations. It is possible to show, from isotopic analysis of fluid inclusions, brines and embedded minerals, that some interbedded salt/clay horizons have remain unchanged since the time of their deposition. This provides evidence that, under certain conditions, rock salt may be unaffected by intrusion of external groundwaters over very long, geological timescales.

- The viability of microbes in the near-field: it is accepted that microbes will be present but unclear whether they are significant. Information from old mines, operational disposal sites (WIPP, Morsleben etc.) might be useful to determine whether populations are viable and could actually impact the integrity of the repository, e. g. by contributing to gas generation or formation of corrosive substances to damage the barriers.

- The significance of disseminated hydrocarbons: a repository will be sited away from large accumulations of oil and gas, but hydrocarbons may be finely disseminated throughout rock salt. Similar to the issue of microbes, information from deep old mines or from cores of deep boreholes (deeply buried salt formations) etc. might be useful to determine whether thermochemical reduction of sulphates is an observed phenomenon on a large scale, so could be an actual risk to the repository, or only a theoretical possibility.

- Material degradation and corrosion: different materials will be used in the construction of waste containers and the engineered barriers, and some of these may degrade or corrode in the highly saline near-field environment. Not all modern materials have an archaeological analogue, but examination of artefacts from old mines could provide bounding limits on what materials degrade and which are stable in both dry and humid saline environments.

4.4.2 Natural Analogue working Group (NAWG)

The Natural Analogue Working Group (NAWG) is active for more than three decades now and represents an international platform for the participants to exchange their experiences in planning and studying and evaluation of analogues for their national repository programmes. Participants meet at biennial workshops presenting and discussing most recent results. The information from these workshops including information about current analogue studies and a publication archive can be found on the new developed NAWG website (http://www.natural-analogues.com/).

Main contributions from the German side to recent workshops were based on the outcomes of the international Salt Club workshop on Natural analogues for safety cases for repositories in salt as described in Chapter 4.4.1. In addition to that the German strategy on the use of analogues has been further developed and some specific aspects have been reported, lately.

In 2013, a new Site Selection Act (Standortauswahlgesetz) became operative in Germany. The aim of this Act is to find a disposal site for high-level waste in Germany in a scientifically-based, transparent process. The geological formations included in this process as potential host rocks will be rock salt, clay and crystalline rock. Important elements in the site selection process will be the safety cases for selected potential repository sites/formations. Due to the German requirements for the disposal of heat-generating radioactive waste /BMU 10/, a safety case needs to demonstrate that containment of the waste within the so-called containment-providing rock zone will be achieved. Therefore, safety concepts are based on the safety functions of containment and to some extent retardation. The key barriers providing these safety functions are the geological formation and geotechnical barriers. Thus, underpinning the integrity of these barriers is crucial, and natural and anthropogenic analogues consequently play an important role, alongside laboratory experiments and process modelling.

This study introduces the top-down approach used to identify relevant analogue studies to be used in the safety case. For a potential repository in rock salt, a systematic analysis was started few years ago and is described in /WOL 15/. Since then, some aspects have been further developed and some new results have become available. /BRA 14/ have compiled detailed reviews for the following NA-relevant topics: the behaviour of competent formations, compaction of crushed salt, composition of fluid inclusions, thermal and mechanical stability of rock salt, impact of earthquakes on a rock salt formation/repository, qualified shaft and drift sealings, iron corrosion, and microbial processes. The reviews include the relevance for the safety case, knowledge from laboratory and field experiments and modelling, and potential natural analogues, with an evaluation including the time frame, uncertainties, limits of application, suitability for communication, open questions and references. Selected new aspects on geomechanics are briefly discussed here.

4.4.2.1 Mechanical stability and self-sealing of rock salt

An important aspect for the disposal of radioactive waste in rock salt formations is the visco-plastic behaviour of the salt. By the convergence process in several 100 m depth, the pore volumes in backfilled areas and in the excavation-disturbed zone will be reduced and, depending on the convergence rate and temperature, completely sealed after a few thousand years. Analogues can be used to demonstrate these properties and the influence of corresponding processes under repository conditions. Analogues from mining and geological analogues are considered to be particularly suitable in this respect.

One example demonstrating the self-sealing capacity of rock salt is the analyses of the post-gas-frac situation at the Merkers site after a rockburst at Volkershausen /POP 07/. After the disastrous event of barrier rupture due to CO_2 expulsion, a time-dependent recovery in the integrity of the mechanical and hydraulic barrier was, at least partly, demonstrated during over a short period of only 18 years. It has to be mentioned that, in addition to the rock burst itself and the associated event of a gas-frac, the subsequent sealing could be simulated by the performed rock mechanical back-analysis of this scenario (for details, see /POP 07/).

The self-sealing of the excavation disturbed zone is also observed in a technical analogue at Asse mine, where a drift was excavated in 1911 and 25-m-long part of it was subsequently sealed by a steal liner and concrete. Permeability measurements around the sealed drift demonstrate that it decreased from approx. 10^{-15} m^2 after excavation (and still today observed in the EDZ of the open drift) to 10^{-19} m^2 today /WIE 03/. The observations of this technical analogue, which covers a significantly larger time frame than laboratory and field experiments, have now been simulated by constitutive models describing the thermo-mechanical deformation of rock salt /HAM 15/, and might consequently serve for the qualification of these models. Similarly, fractures observed in the Sigmundshall salt mine and probably originating from the formation of the salt dome and its tectonic situation are also completely filled with secondary halite crystals, and have been efficiently, hydraulically sealed (Fig. 4.21, middle).

Another illustrative example showing the convergence process is the embedding of tools or other mining materials as, for example, observed in the Hallstadt salt mine in Austria for more than 3000-year-old material (see Fig. 4.21, right). Examples like this might help to visualize and communicate the convergence process and the principle of containment of the waste in rock salt, particularly to non-technical audiences.

Fig. 4.21 Technical analogues from mining and geological analogues for convergence and self-sealing of rock salt

A drill core with sealed rock salt after gas-frac (left, /POP ´07/); fractures at the 350 m level in the Sigmundshall salt mine (Bokeloh, middle, /HAM 12/) and an old wooden staircase, 1300 BC, Salzkammergut (Austria, right)

The impact of an earthquake might impair the integrity of the host formation and has to be addressed in a safety case. Although a repository site in Germany will certainly not be located in a seismically very active area, there is a need to demonstrate that the containment-providing rock zone will not be jeopardized by the dynamic strain of an earthquake and keep its safety function. Besides geomechanical model simulations, technical analogues, namely rock bursts, have been identified as strong arguments to estimate the effects of an earthquake on rock salt. Therefore, twelve salt mines in which rock burst have occurred during the last century have been compiled /MIN 10/. Investigations showed that the geological barrier of rock salt and salt clay had retained its integrity against overlying aquifers in all cases. From the analyses of the rock bursts, it became clear that they provide a significantly higher dynamical strain compared to that from an earthquake. A general conclusion, which is discussed in more detail in /MIN 10/, is that a repository in rock salt is earthquake-resistant for a sufficiently thick salt barrier.

4.4.3 Natural analogue study Ruprechtov (CZ) - An experience report

In cooperation with Czech organizations SURAO and UJV the information, knowledge, and experiences gained during the investigations at the natural analogue site Ruprechtov, in Czech Republic has been compiled in an experience report /NOS 14/. Besides a brief overview on the different roles of analogues in national repository programmes and the evolution of analogue application in safety cases the intentions and objectives of this report were to

- compile and critically discuss the decisions regarding the selection of the Ruprechtov site as a natural analogue,
- classify the Ruprechtov site with regard to the type of uranium accumulation,
- display the iterative steps, decisions and evolution of knowledge during the investigation of the site,
- describe the experiences obtained, particularly in the selection and application of experimental laboratory and field methods,
- outline the scheme by which these methods have contributed to understanding and characterizing the main features of the site,
- illustrate the main findings relevant for a safety case for a radioactive waste repository, and
- outline recommendations for future R&D from the lessons learned.

In the following the main aspects of the report are briefly mentioned and the lessons learnt are summarized.

4.4.3.1 Main aspects of the report

The Ruprechtov project was initialized in 1995. At that time the preferred options for the disposal of heat-generating radioactive waste were repositories in a salt dome in Germany. At that time of scant knowledge and ideas were available and the concept of a safety case had not yet been implemented.

For the German repository programme, at the beginning of the 1990s a national expert group discussed the relevance and application of natural analogues for the assessment of the long-term safety of a radioactive waste repository and identified major topics for their use. One of seven identified topics concerned nuclide retardation in the overburden, especially the interaction of radionuclides (uranium and thorium) with Quaternary and Tertiary sediments under central European climate conditions /STE 96/. Based on existing knowledge of the sedimentary basin in Northern Germany, specific questions have been raised about the function of the overburden as a barrier for radionuclides, the corresponding processes such as dispersion, sorption and precipitation, as well as the role of organic matter, colloids and microbes. The objective was to increase the understanding of fundamental transport and retardation processes under complex natural conditions. On that basis the Ruprechtov site had been selected as analogue site.

The report mentions the knowledge about uranium deposits and natural analogue studies at the beginning of the Ruprechtov project, it describes natural uranium containing systems, particularly the different types of uranium deposits and in relation classifies the uranium accumulation at Ruprechtov, and it discusses the applied stepwise approach of the Ruprechtov study with its advantages and disadvantages.

Special focus was put on the description of the different methods applied including challenges and problems, which appeared during their application in the project. It was distinguished between drilling methods, drill core and GW-sampling methods, methods for characterizing geological parameters, in-situ measurements, chemically based analytical methods, micro- to nanoscale analytical methods, isotope investigation methods and modelling tools.

It is then in detail described in the report how different methods have been applied, in order to understand key aspects of the Ruprechtov site with relevance to scientific and safety related issues. For all key aspects the output of each method as well as the interpretation and interplay of the different methods in comprehensively describing the key aspect is illustrated. Therefore, standardized flow schemes were developed as shown exemplarily for the investigation of uranium migration processes in Fig. 4.22.

In the original experience report these schemes are directly linked to and to the descriptions of each method, thus, easily allow finding details and experiences for the methods applied in the Ruprechtov project. All these methods are described in formatted tables. As an example, the method for U(IV)/U(VI) separation in sediment samples and groundwater is listed here in.

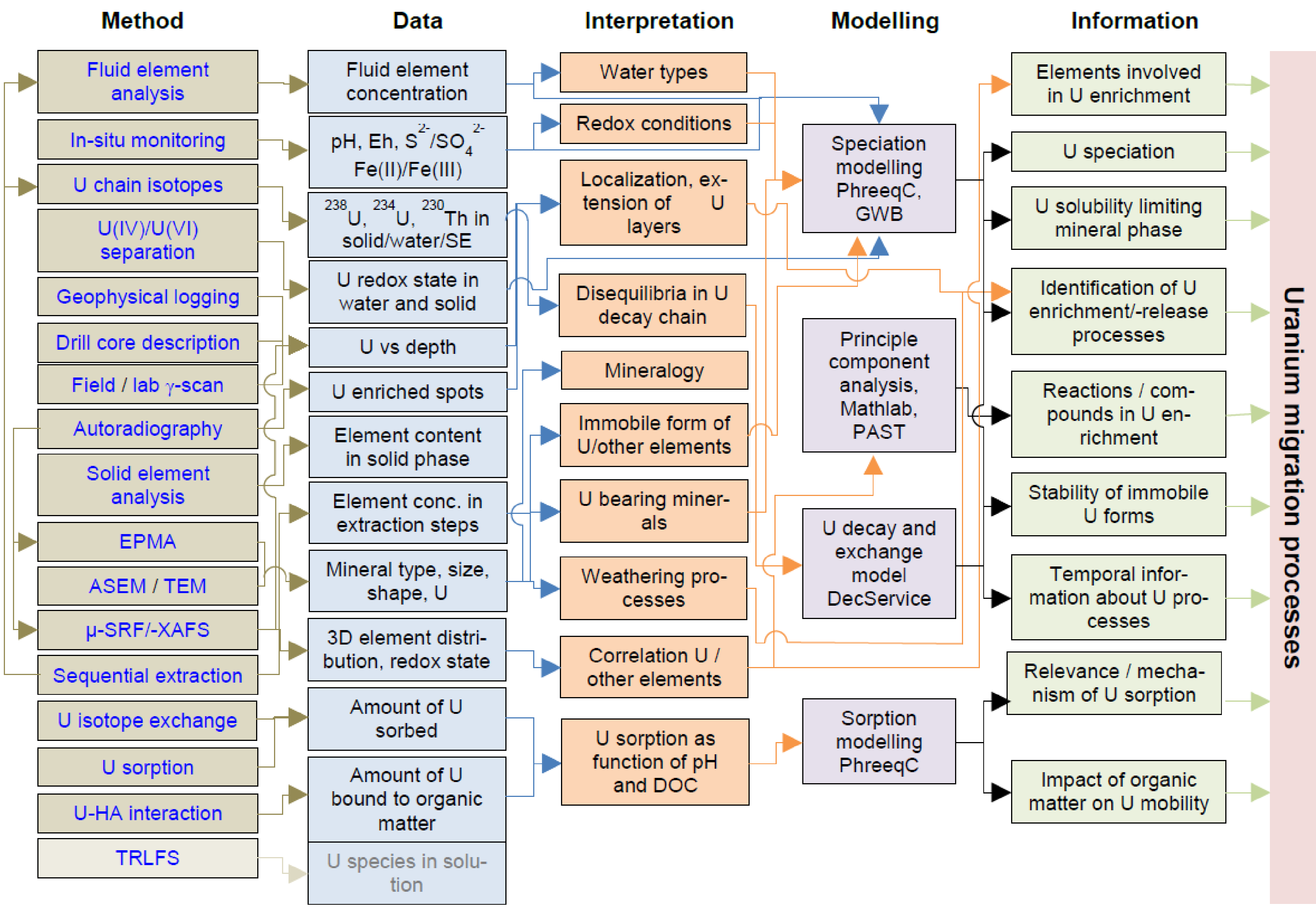
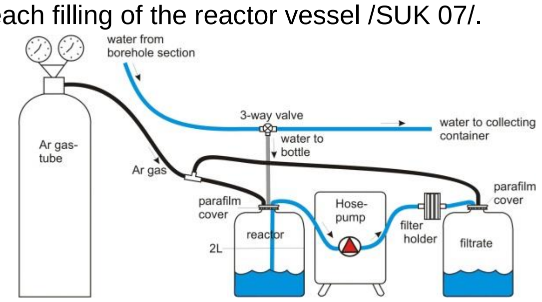
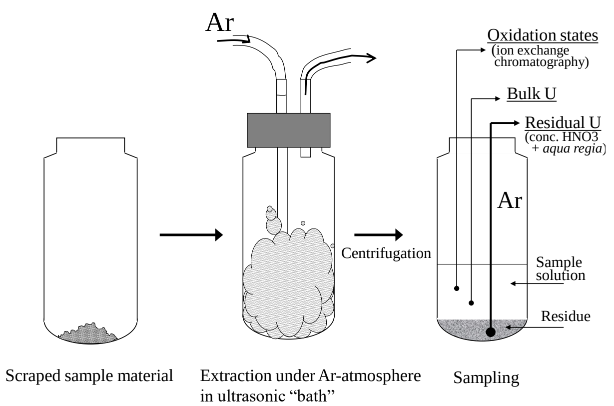


Fig. 4.22 Evaluation scheme with methods, data, interpretation and modelling for uranium migration processes

Tab. 4.3 Method No. 4.1: U(IV)/U(VI) separation

Name of method	U(IV)/U(VI) separation
Application in the Ruprechtov project	Analysis of U oxidation states in sediment samples and groundwater coupled with analysis of the $^{234}U/^{238}U$ activity ratio.
Device(s) / method(s) used / applied	1. α-spectrometry 2. Wet chemical separation
Brief description of the functioning	<u>Sediment:</u> U(IV)/U(VI) distribution is determined by applying a wet chemical method slightly modified from /ERV 96/. Uranium extraction from sample material is done in the 4 M HCl-0.03 M HF mixture under Ar atmosphere. U dissolution yield was 50-90 %. Insoluble U was considered U(IV). Extraction solution with U(IV) and U(VI) is fed into a Dowex 1x4 anion-exchange column where U(VI) is sorbed while U(IV) passes the column in the first 20 ml. Sorbed U(VI) was eluted with 20 mL of 0.1 M HCl. Separation is quantitative and no significant overlap of U(IV) and U(VI) fractions has been observed in the tracer experiments. U(IV) and U(VI) with their $^{234}U/^{238}U$ activity ratio were measured with α-spectrometry. <u>Groundwater:</u> U(IV) and U(VI) are separated from groundwater during sampling using a U(IV) specific co-precipitation technique (NdF_3-precipitation) which keeps U(VI) in solution /AND 83/. NdF_3 precipitate was filtered and the filter and filtrate water analysed for U. The U concentrations show how much occurs as U(IV) relative to U(VI).
State-of-the-Art and new developments	The methods applied at Ruprechtov are rarely used but have theoretically sound basis /AND 83/ and /ERV 96/. New developments have been done in controlling iron induced interferences during uranium extraction and using the $^{234}U/^{238}U$ ratio as a tracer in monitoring U(IV) and U(VI) separation. Significantly higher $^{234}U/^{238}U$ activity ratio in U(VI) fraction can be considered an evidence of a success of separation.
Output of the method	The method yields the U(IV)/U(VI) distribution in sediment and groundwater samples.
Objective(s) of application in the Ruprechtov project	Identifying the redox state of U compounds in sediment and groundwater and studying the option that the reduction of U(VI) to U(IV) controls U immobilization and accumulation in the sediment.
Practical procedure and experiences in the field	Solid sampling: No specific sampling was done, but see comment under “Experiences”. Groundwater sampling (see figure below): The equipment consists of two plastic containers (HDPE), the reactor vessel where precipitation takes place and the container for collecting the filtrate. A Nucleopore polycarbonate filter (ϴ 47 mm, 0.40 µm) placed in a plastic filter holder was used for filtration, and a peristaltic pump served to pump the solution through the filter. Pumping was done under Ar atmosphere. Groundwater collection, NdF_3-precipitation and filtration. A bypass was arranged to accommodate disposal of the water between each filling of the reactor vessel /SUK 07/.  *Equipment setup for field separation of U(IV) and U(VI) in GW*

Applicability	The method is applicable if enough uranium is available for the measurement. In practice for α-spectrometry > 1 μg and for HR/MC ICPMS > 0.1 μg are needed to get statistically good result.
Limits of application	The limitation is given by the amount of uranium (see above).
Uncertainties / accuracy (devices, methods, evaluation procedure)	Analytical uncertainty is due to α-counting statistic. Main uncertainty is related to the material itself and particularly the iron in the material because possible post-sampling oxidation of the material increases Fe^{3+} which can disturb uranium redox-state during the extraction by oxidizing U(IV).
Method specific to defined boundary conditions	The method can be applied to all geological media. For solid samples higher amounts of redox-sensitive elements like iron (s. above) might perturb the measurement; for groundwater, undisturbed samples (without contact to the atmosphere) are needed.
Experiences (pos. / neg. what to avoid)	- Solid: In order to avoid oxidation of redox sensitive samples it is recommended to perform U(IV)/U(VI)-separation in the field directly after drilling and identification of U-rich areas by field γ-spectroscopy - Water: To avoid contact with oxygen (oxidation) Ar-flooding of the borehole some minutes before sampling was successful For filtration of groundwater and U(IV)/U(VI)-separation in the field pumps with enough (continuous, stable power and long-term electricity supply are preferable
Effort, comments	- Sample preparation, analysis and measurement for U isotopes take about 2 days depending on U concentration. Data are derived from α-spectrometry by standard procedures. Analysis of more than one sample is recommended to give statistically sound interpretation - Most part of the costs consists of consumed time in analytical work and interpretation. Additional costs come from materials and chemicals. Consequently, the price per sample varies a lot an average being around 500 € for solid samples and 100 € for water samples
Links, references, other sources of information	University of Helsinki, Department of Chemistry, Laboratory of Radiochemistry: http://www.helsinki.fi/kemia/radiokemia/english/
Picture of the device	 Laboratory device for U(IV)/ U(VI) separation in the solid

In retrospect, the Ruprechtov study has provided a great deal of experiences, knowledge, know-how and skills. The lessons learned are summarized in the following.

4.4.3.2 Lessons learned

The Ruprechtov project has demonstrated that understanding the evolution of a geological site (past and future) and evaluating the long-term behaviour of a deep repository require a broad and well-founded knowledge of the geological conditions (regional and local) including all geo-historical processes. This makes up the scientific basis for site investigation and the interpretation of genetic-mineralogical, geochemical, hydrological and other important geo-parameters. The overall geological knowledge together with the findings from the investigations provide the information needed for a first, model-like assessment of the long-term performance of geological barriers as part of repository systems.

The outcome of this project has confirmed the association of specific uranium-bearing minerals with different genetic types of uranium accumulation and different stages of the genetic evolution of the geological system. In addition, the interpretation of the findings from petrographic, mineralogical and microscopic studies have given distinct indications not only for uranium migration but also for uranium accumulation and sorption processes in argillaceous formations under the present environmental / climatic conditions. In general, it was proved that argillaceous sediments, even close to surface, can contribute essentially to the retention of uranium for long (geological) periods of time. Specifically, in the case of the Ruprechtov site, lignite-bearing sediments are the source for a microbial milieu which provides long-term reducing conditions and the efficient immobilization of uranium.

The performance and the success of a research project of this kind depend significantly on the availability of professional experience in the issues concerned and scientific knowledge. This has been demonstrated to some extent by the literature survey performed on relevant publications and reports covering subjects such as the use of natural analogues in radioactive waste disposal research, the formation of natural uranium deposits under different geological conditions and the basics of the national and regional geology. The analysis and the evaluation of around four hundred documents made it possible to view the investigation results in the context of the actual state-of-the-art in uranium mineralogy and geochemistry. All of this provided the information required for defining more clearly the scientific goals over the course of the project and, respectively, for outlining the overall investigation results.

One major advantage from the beginning was in a broader sense the easy accessibility of the site, which should be a prerequisite, because the need for discussion / negotiation / explanation with local responsible persons is inescapable. On the other hand, the high-quality kaolin at low depth, which meant that it was easy to mine, led at the outset of the project to different interests being held by the kaolin mining company because of economic planning. However, through the negotiation of clear arrangements and good relations between the scientists and the mining company, both sides were able to perform their work as intended. In a few cases, these arrangements limited the selection of a borehole location and also led to the abandonment of a few boreholes, but the relevant information was always communicated in advance. The interdependency with the kaolin mining company also had positive aspects, e. g. groundwater wells constructed by the kaolin mining company were made available for use in the study and vice versa, hydraulic and geochemical information from the Ruprechtov study was also integrated in the environmental impact assessment of the kaolin mining company.

A further argument for the decision to choose this location was the limited extension of the Tertiary basin suggesting a system with limited complexity in its geological evolution. During the detailed investigations this assumption turned out to be unjustified, since the results clearly showed that uranium enrichment happened through many different processes over different time scales. Indeed, this posed an additional challenge but did not constrain the investigations.

Furthermore, the objective to investigate uranium retention in the sandy argillaceous inclusions / layers in the Tertiary basin was achieved, because the uranium enrichment turned out to be very stable and no traces of either a uranium plume or uranium immobilization could be found in any of the investigations. This characterizes the location to be a strong analogue for a long-term stable geochemical environment being the cause of the high stability of the immobile uranium. However, this fact did not allow the study and modelling of the migration of uranium on a pathway through the sedimentary environment, which had also been one of the initial ideas.

An additional aspect of choosing the site / location was the objective to study organic material, particularly sedimentary organic material as a source of organic colloids such as humics or fulvics, which might act as a carrier for radionuclides. This would have been of interest for the German scientists, because high concentrations up to 200 mg C/L of humic colloids have been observed in the overburden of the Gorleben site, considered in the past for hosting a HLW repository. The investigations at the Ruprechtov site showed a very low availability of sedimentary organic matter for degradation and consequently only low concentrations of dissolved organic carbon (humic colloids) in the groundwater, limiting its value as an analogue for the specific situation at Gorleben. Nevertheless, valuable contributions have been made to an increase in knowledge on the interrelation / interaction of organic and inorganic carbon. Moreover, it indicates and gives some confirmation, as observed in several other natural analogue studies, that the impact of colloids on a potential radionuclide transport in many natural systems is limited.

The whole study was performed stepwise, which is necessary for such an analogue site investigation. This investigation strategy is a key prerequisite for maintaining flexibility. The stepwise procedure caused the relatively long duration of the project, which, however, is also revealed by experiences from other analogue site investigations of this kind; around 15 years were necessary to yield full site understanding. On the other hand, this approach made it possible to plan further steps thoroughly and according to the real needs and requirements, which was economically and scientifically of benefit. Besides specific investigations, each step also allowed the adoption or modification of technology, e. g. drilling technique or the kind of instrumentation and the use of analytical equipment. Moreover, it allowed, for example, the identification of key features of the groundwater and sediments, which needed to be carefully accounted for in the following steps of the project. These findings then led to a change / optimization of (i) sampling, (ii) sample handling and (iii) experimental procedures. This concern, for example, the redox sensitivity or high heterogeneity on low spatial scale of sediment samples from the uranium-bearing layers. The former aspect provoked an improved sampling method, providing rapid isolation of drill core material from the ambient atmosphere directly after drilling as well as the application of experimental procedures under anaerobic conditions.

This redox sensitivity of the drill core material led to the decision to perform some of the analysis directly on-site instead of later on in the laboratory. One example is the uranium(IV) / uranium(VI) separation, which is, of course, very sensitive to oxidation by atmospheric oxygen. Therefore, a mobile glove box was applied to perform U(IV)/U(VI) separation under Ar atmosphere on selected samples directly after drilling. As expected, the results showed an extremely low fraction of the oxidized form U(VI). On the other hand, a drawback of this decision was that no information about the absolute U-content in the sample was available directly after drilling. Unfortunately, the selected core was one in which the uranium enrichment was rather low, leading to low U signals. This is a consequence of the high heterogeneity (also in uranium content) on a relatively small spatial scale.

For each of the methods applied during the Ruprechtov study, specific positive and less positive experiences were gained, which were described in “method tables”.

Some specific drawbacks should also be mentioned. The low-permeable system at the site with low water supply in some of the boreholes represented a special challenge for groundwater sampling and in-situ measurements. It was not possible to completely change the well volume in some of the groundwater wells, because the inflow was too slow. In such a case, just to “optimize” the system, borehole pumping was performed several days before a sampling campaign. The problem of confidence in the results of Eh measurement has been discussed several times. It was observed that never Eh-values as low as those measured with the in-situ probe in the borehole were reached. Moreover, each pumping in the near-surface boreholes could be recognized by an increase in the in-situ Eh-value. Several hours up to a few days were needed to receive a stable and reproducible signal which was used for interpretation and modelling.

The study also showed that the methods adapted have been restricted in some aspects, so that not all questions could be answered completely. One example concerns the identification of low size U-bearing minerals (diameter below 1 µm). From mass balancing it is obvious that part of uranium will be enriched in the submicron phases. Therefore, within the last stage of the project, we applied transmission electron microscopy (TEM), which actually allows detection down to a nanometer scale. However, this effort failed, particularly due to the difficulty of selecting the correct samples on that small spatial scale. No uranium phase could be identified. Such an investigation should have been started earlier and more effort should have been dedicated to it.

Uranium speciation in solution was investigated using U(IV)/U(VI) separation. This method was optimized during the project but also requires a great deal of effort and logistics. We succeeded in measuring U(IV) and U(VI) fractions in three boreholes, which agreed well with modelling results. However, to underpin these results more analyses using a larger network of boreholes correlated with in-situ and chemical parameters would be necessary.

Some development work was also dedicated to the Time Resolved Laser Fluorescence Spectroscopy (TRLFS), with the final aim of identifying U(VI) species. A particular aim was to prove the existence of ternary uranyl carbonato complexes in a typical groundwater from Ruprechtov. We have been successful in identifying four uranyl species, including $Ca_2UO_2(CO_3)_3$, in synthetical Ruprechtov water and determining their lifetimes. However, the step to directly measure a sample taken from a Ruprechtov well with relatively low uranium concentration is still a challenge and was not performed within the project.

With respect to the safety case, evidence has been achieved through several different observations that a sedimentary formation may act as a strong long-term barrier for uranium migration. Similar to the findings from the Tono study, microbial sulfate reduction involving organic matter degradation is inferred to be the dominant buffering reactions that has maintained the strongly reducing conditions in the sedimentary uranium deposit over time frames of hundreds of thousands up to million years and efficiently immobilized uranium. The results support the assumptions that under these conditions maximum U concentrations are determined by amorphous uraninite, which is a frequent assumption in safety assessments and herewith underpinned by analogue information.

To perform the project in the way in which it was done was only possible because of co-operation with international experts and working teams. Such a study requires not only knowledge and expertise in different disciplines such as geology, mineralogy, hydrology, hydrogeochemistry and microbiology to establish a broader view on the topic, but also specific technical experience such as application and evaluation of isotope methods or use of specific modern and state-of-the-art micro-/nano-analytics. A particularly important aspect of this co-operation was method-development and testing. This comprised, for example, colloid sampling under undisturbed conditions, first applied to natural samples and further development of µ-XRF and µ-XANES as well as the application of modern isotope analyses such as the study of $\delta^{34}S$ signatures to identify relevant processes in the field.

All of these methods are important for the investigation of a potential repository site including laboratory and field experiments.

4.4.4 Analogues for a repository in a clay formation

Natural analogues are natural (from specific site or similar type of rock) or artificial material occurrences of e. g. metals or cements, which are similar to the materials used in the repository. For example, analogues for the clay formation may be marine or lacustrine sedimentations and/or deep natural bentonite occurrence with or without inclusions (metal, wood), external influences like changing temperatures/pressures due to volcanic or glacier influences and different hydrochemical boundary conditions (e. g. salt water, alkaline water). The main advantage of analogues is their longevity (up to Millions of years), large spatial extension, structural complexity of the geological / hydrogeological environment and the different influences they had been exposed (e. g. temperature due to magma intrusion, gas pressure due to natural gas resources in or covered by clay formations/technical gas storage in underground reservoirs, transport due to substances in the pore water of the rock from today's distribution of tracers, pH, redox). Therefore, they can support prognoses of the future evolution of processes and materials behaviour expected in repositories under changing conditions.

A significant contribution to the safety assessment of a nuclear waste repository can be expected from the natural analogues with regard to following aspects:

- Expanded system/process understanding and broad database will afford an opportunity for the
  - identification of key process and definition of main process factors,
  - a more plausible and reproducible argumentation of conservative data selection,
  - the detection of weak points within repository design / used materials, and their interaction to each other.
- Systematic, reproducible and transparent approach of FEP:
  Testing of completeness and classification into influencing and not influencing processes.
- Definition of probable scenarios as well as scenario analysis with estimation of more or less likely occurrence.
- Part of the verbal-argumentative stepwise approach based on facts (pictures and handouts) and qualitative / semi-quantitative arguments, which can`t be disproved and should give confidence in the materials long term behaviour.
- Identification of information gaps and future work.

- Prognoses of the future evolution of repository materials (especially materials of container, geotechnical barriers and host rock), which can be only partly be investigated by experiments (in-situ, laboratory) or computer models.

Analogues cannot support these goals per se, but they can help to study specific processes, which might affect important functions of repository materials. Therefore, in overall, natural analogues provide an important input for the safety case or rather the safety concept, which needs to demonstrate that containment of the waste within the so-called containment-providing rock zone will be achieved by means of the geological formation and geotechnical barriers.

4.4.4.1 Study approach

In this study, which is described in detail in /FAC 18/, analogues for a repository in clay formation had been compiled with respect to support the safety case for a potential German repository for heat generating waste in clay. The approach was performed in three stages.

The first stage is based on the repository and safety concept, which has been developed within the German R&D project ANSICHT. According to the safety concept /RUE 14/, the containment of the radioactive waste is primarily achieved by hindering the radionuclide transport by chemical and physical processes resulting from positive properties of the clay host rock in combination with geotechnical barriers. This primary goal is achieved by a set of goals listed in the safety concept. A shortened outline of this set of safety goals is given in the following and is numbered for clarification: A detailed description can be found in /RUE 14/.

I.1. Integrity of containment providing rock zone (CPRZ)
The containment providing rock zone (CPRZ) stays intact over the whole assessment period and its barrier function is neither affected by internal or external events or processes.
This is a high-level goal directly following a requirement from the Safety Requirements Governing the Final Disposal of Heat-Generating Radioactive Waste /BMU 10/. Natural analogues cannot support this goal per se, but only help to study specific processes which might affect the barrier function of the CPRZ. These might be either processes induced from the repository itself or natural processes occurring also without the existence of the repository. The

most relevant processes are considered separately in respective additional goals below.

I.2. Limitation of radionuclide transport through the CPRZ

Transport of pollutants is hindered and retarded after their mobilization from the waste by chemical und physical processes in the CPRZ.

a. The limitation of advective transport, which is achieved by the limitation of water flow due to a low permeability of the host rock and geotechnical barriers.
b. The limitation of diffusive transport, which mainly is achieved by small values of diffusion coefficients, high sorption capacity and low solubility limits in the clay backfill and clay rock. The buffer capacity of the host rock preserves the positive retardation properties over the full assessment period.
c. The restoration of the initial low permeability. Those parts of the host rock which are disturbed by the excavation of the mine are self-healing in combination with the geotechnical barriers and backfill in a way that the initial low permeability of the CPRZ is restored.

I.3. Criticality of the waste can be excluded for the whole assessment period.

This goal is a demand from the safety requirements /BMU 10/. According to the procedure developed in the preliminary safety case for Gorleben (VSG), the assessment of criticality is treated separately from the long-term assessments of the host rock integrity and the radiological consequences.

I.4. Reduction of consequences from and probability of human intrusion.

The optimization of the repository with regard to human intrusion is a second-tier goal from the safety requirements /BMU 10/, that has to be considered in the optimization process, only.

I.5. Limited temperature of the host rock

The maximum temperatures in the host rock are limited to a value that the barrier function of the host rock is not ineligible affected.

High temperature might result in a change of mineral phases in the clay host rock. The effect of an elevated temperature on the different rock properties might be investigated in analogues where the host rock or comparable rock types were exposed to elevated temperatures in the geological past, e. g. from magma intrusion

I.6. Enabling waste container recovery

The waste containers can be handled for at least 500 years after closure to enable a potential recovery.

I.7. Limitation of gas pressure development

The gas pressure development in the repository is limited in a way that the integrity of the host rock is neither affected by the gas pressure nor by the gas flow through the rock.

High gas pressures or gas flow might result in the fracturing of the host rock which potentially is a damage of the CPRZ integrity. Clay formations which are under a pressure load from gas can be found in natural and technical environments. Examples are natural gas resources in or covered by clay formations as well as technical gas storage in underground reservoirs. Both cases can be potentially suitable to serve as analogue for gas pressure effects to and gas transport processes in clay formations.

I.8. Limitation of microbial processes

Microbial processes should be limited as much as possible.

I.9. Limited host rock deformation

Deformation of the host rock should be limited as much as possible, e. g. by back-filling the void spaces with swelling material.

I.10. Resealing of drift pathways

Potential pathways along the drifts should be resealed to avoid advective transport processes.

Those parts of the host rock which are disturbed by the excavation of the mine are self-healing in combination with the geotechnical barriers and backfill in a way that the initial low permeability is restored.

Furthermore, as described above, analogues can contribute to the description of the behaviour of materials under repository conditions. Various materials are emplaced in a repository for heat generating waste in clay. These might either be materials emplaced together with the waste, for the construction of the mine or for the sealing of the mine after emplacement. Two different repository concepts were described in the AnSichT project. These are the borehole emplacement concept /LOM 15/ and the drift disposal concept /JOB 15/. In the following the major part of the emplaced material types is listed. The waste itself is not regarded.

Steel: The largest amount of steel is used for the container and the borehole liner: In the borehole disposal concept, the containers are mainly made from fine grained steel, the liners from cast iron. In the drift disposal concept, the container (Pollux) are made from cast iron in the outer and fine-grained steel in the inner parts. In both concepts the installations to hold the waste assemblies within the containers are made from stainless steel.

Concrete: The largest part of the concrete foreseen in the repository concepts is support for all drifts and openings in the repository mine. The thickness of the support is currently estimated to be between 0.3 to 0.5 meters. Concrete is also used in all sealings as abutment. The abutments have a length of 3 to 5 m depending on the type of sealing.

Bentonite will be used as buffer material in the near-field, for the sealing elements and possibly as additive to the backfill. Apart from sealing locations, drifts and openings will be backfilled with clay-based material.

Other materials of lower, but significant amount are sand (backfill between inner liner and container), crushed hard rock (backfill e. g. in the lower part of the shaft column), asphalt (potential sealing material) and polyethylene (used as shielding material in the container). They have not yet been investigated for their potential to be studied by natural analogues.

In the second stage available natural analogue studies have been compiled and evaluated with regard to their contribution towards the safety goals and/or the behaviour of materials in the repository described above. Until now 29 analogues had been included and analysed in the document. Their documentation has been done in condensed form to get a short overview about the potential of provided information, which might be helpful for the safety case. The information of documented analogues refers to different environments and external impacts. Depending on performed investigation within the analogues area, there is a different amount of available data and data quality. Some analogues are just of describing nature like “China” or “Inchtuthil”, others contain a lot of data (e. g. boreholes, groundwater sampling / analysis, modelling, tracer experiments).

The analogue studies, which have been included in this review are listed in the first column of Tab. 4.4. The correlation to the safety goals and the key materials intended to be used in a repository in a clay formation in Germany are indicated by a cross in the respective field of the matrix.

Currently analogue information to the safety function “Integrity of CPRZ” and “Transport of radionuclides” can be often found. Information about “Microbial Activity” and “Temperature Effects” are not common and such of “Development after Deformation”, “Criticality”, “Gas Pressure Development” and “Resealing of Pathways” are very rarely.

Tab. 4.4 Overview of documented analogues and relation to safety goals and materials (marked by x) used

L.I	Safety Objectivs	I.1	I.2	I.3	I.4	I.5	I.6	I.7	I.8	I.9	I.10	II.1	II.2	II.3	II.4	II.5
	Sites	Integrity of CPRZ	Transport through CPRZ	Criticality	Human Intrusion	Temperature - Host Rock	Waste Container Recovery	Gas Pressure Development	Microbial Processes	Limited Deformation Host Rock	Resealing of Drift Pathways	Steel	Concrete	Bentonite	Clay Backfill	Other Materials
1.1	Bangombe, Gabon		x	x										x	x	x
1.2	Barra, Spain	x	x			x						x		x	x	
1.3	Boom Clay (Mol), Belgium		x											x	x	
1.4	Broubster, Scotland		x											x	x	x
1.6	Busachi, Italy	x				x				x	x			x	x	
1.7	Cabo de Gata (Almeria), Spain	x												x	x	
1.8	China	x							x					x	x	x
1.9	Cigar Lake, Canada	x	x						x			x		x	x	x
1.10	Disko Island, Greenland											x				
1.11	Dunarobba, Italy	x						x	x					x	x	x
1.13	Heselbach, Germany		x											x	x	
1.14	Isle of Skye, Scotland	x	x			x								x	x	
1.15	Kato Moni, Cyprus	x	x										x	x	x	
1.16	Kinekulle, Finland	x				x				x				x	x	
1.17	Kronan cannon, Sweden	x	x											x	x	x
1.18	Kushaym Matruk, Jordan	x	x			x						x	x	x	x	x
1.19	Littleham, UK		x					x						x	x	x
1.20	Loch Lomond, Scotland		x											x	x	
1.21	Luzoni, Philippines								x				x	x	x	
1.22	Madeira Abyssal Plain, Portugal		x						x					x	x	x
1.23	Marqarin, Jordan	x	x						x	x	x		x	x	x	
1.24	Natural Tracer profiles in argillaceous formations	x	x													
1.25	Oklo, Gabon		x	x		x			x					x	x	x
1.26	Opalinus Clay, Switzerland	x	x							x	x			x	x	
1.27	Orciatico, Italy	x	x			x				x	x			x	x	
1.28	Parsata, Cyprus	x	x			x								x	x	
1.29	Searles Lake, California	x												x	x	
2.1	Arch. Metal: Inchtuthil, Scotland											x				
2.2	Arch. Cement: Hadrian’s Wall in Scotland												x			

In a third stage the analogue studies were analysed with respect to their contribution to all features, events and processes (FEP) compiled for a repository in a clay formation. FEP are used for a systematic, comprehensive and consistent approach for derivation of scenarios to be regarded in long-term safety assessment, thus increase transparency and reach credibility (see Chapter 2). In addition, the German Site Selection Act ("Standortauswahlgesetz" 2013) requires a scientifically-based, transparent process to find a disposal site for high-level waste in Germany. One basis for that is a FEP catalogue. FEP for a German repository in a clay formation were derived in the project AnSichT /STA 15/. Exemplarily, the FEP catalogue compiled for a potential site in Southern Germany was used here. FEP are separated into process and component FEP, see Tab. 4.5. Altogether 68 FEP are compiled in the catalogue. The decision on these FEP had been done under consideration, that the repository programme in Germany is still in a pre-siting stage.

For each analogue study a table with those FEP, which the study can contribute to, is contained in the documentation. In addition, all analogue studies are listed in a matrix together with all FEP and correlations are indicated. This Excel table contains information about the FEPs, the analogues site names and numbers. Therefore, a searching and illustration of certain information is possible. Currently the table contains about 180 data set entries. This Excel table can be found in /FAC 18/.

Tab. 4.5 FEP catalogue derived from the project AnSichT

COMPONENT FEP	PROCESS FEP
Waste form and cladding	25 Vertical movements of earth crust
01 Waste form (matrix)	26 Orogeny
02 Spent fuel container	27 Crustal deformation
03 Other disposal container	28 Graben formation
Buffer / Backfill	29 Magmatic, hydrothermal activity
04 Buffer	30 Metamorphism
05 Backfill	31 Erosion
06 Migration trap/seal	32 Sedimentation
Seals / Plugs	33 Climatically induced heat flow
07 Drift seals	34 Atmospheric precipitation input
08 Shaft seals	35 Trans- / Regression
09 Technical installations	36 Foreland glaciation
10 Drift lining	37 Subglacial channel formation
11 Shaft lining	38 Meteorite impact
Gases, Solutions, Corrosion Products	39 Corrosion of spent fuel
13 Corrosion products in the repository	40 Corrosion of glass
14 Repository solutions	41 Corrosion of cement
15 Repository gases	42 Corrosion of metal
Geological Units	43 Hydrogen induced embrittlement
18 Host rock	44 Radiation induced embrittlement
12 Excavation damaged/ disturbed rock zone	45 Dissolution, trans-, neoformation of clay minerals
21 Adjoining rock	46 Dissolution, trans-, neoformation of other minerals
Gases and Solutions	47 Chemical alteration of organics
19 Host rock solutions	48 Microbial processes
20 Host rock gases	49 Swelling, shrinking of clay minerals
22 Adjoining rock solutions	50 Swelling, shrinking of concrete
23 Adjoining rock gases	51 Convergence
Boreholes	52 Heat flow
16 Above-ground exploration boreholes	53 Thermal expansion, contraction
17 Under-ground exploration boreholes	54 Phase transitions
Biosphere	55 Stress propagation
24 Surface water	56 Solution / gas flow
	57 Dispersion
	58 Diffusion
	59 Dissolution, emission of gases
	60 Migration of bitumen
	61 Radioactive decay, ionising radiation
	62 Induced radioactivity
	63 Radiolysis
	64 Ignition of Gas Mixtures
	65 Sorption, Desorption
	66 Complexation
	67 Colloid Formation, Filtration
	68 Thermochemical sulphate reduction

An overview how many of the investigated analogue studies contribute to respective FEP is shown in Fig. 4.23, where exemplarily for the process FEP the number of analogue studies, supporting the FEP are shown. It became obvious, that most information refers to transport mechanism, while there are data lacks in some topics e. g. “Convergence” and “Corrosion of Glass”. The current review would help to perform in a next step a targeted search of further existing analogue studies with respect to those FEP, where not yet suitable analogues were identified.

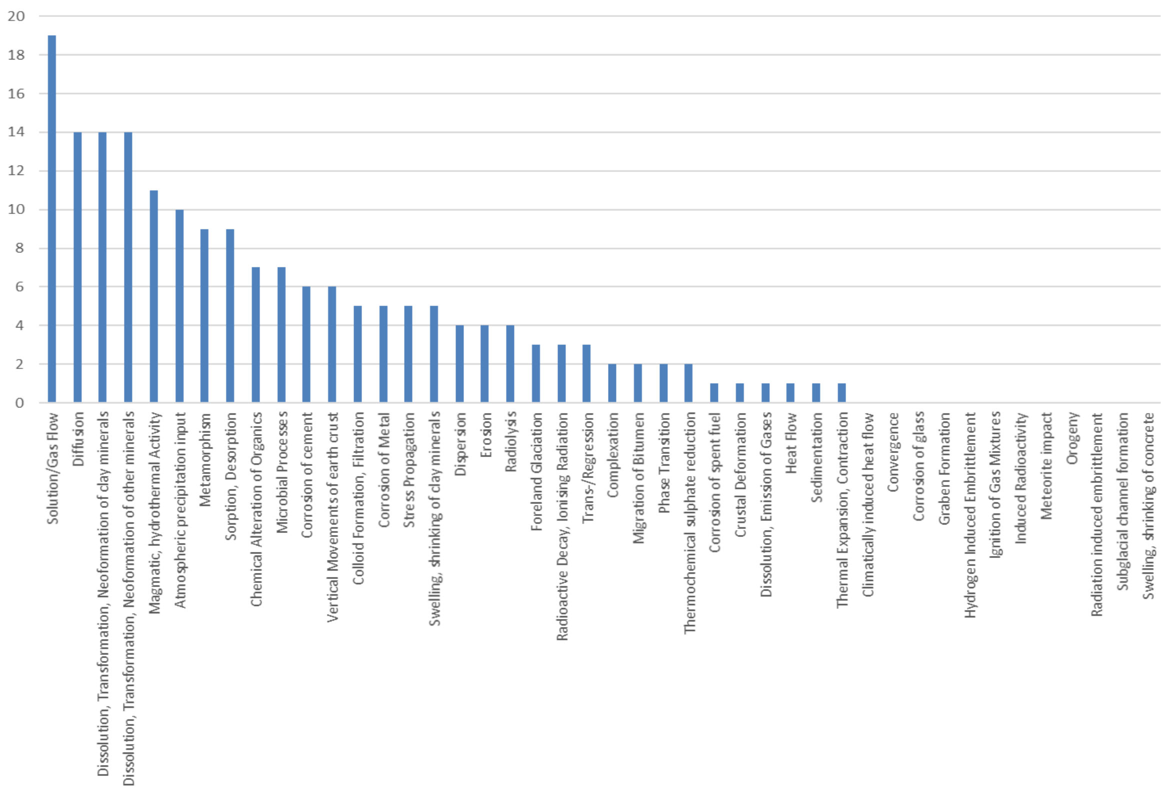


Fig. 4.23 Number of analogues with potential benefit for the different FEP

One example of analogues documentation in the prepared document is given in the following (Chapter 4.4.4.2). Each documentation contains an introductory section, followed by the sections with information about the localisation and a description of the study, a brief description about the investigation, a compilation of the major outputs, the list of FEP, which are supported by the analogue study and the references providing more information about the analogue study.

4.4.4.2 Analogue of Kushaym Matruk (Jordan) - example of the documentation

The site presents several interesting features, like understanding cement hydration, organic matter transformations, migration of transition metals and temperature effects on materials. As an example, the behaviour of clay minerals in the presence of alkaline fluids can be explored. The site is of particular interest, because the biomicrite clay content is significantly higher than in other Jordan sites (Maqarin, Daba, Siwaqa, Suweileh). In addition, there is a direct contact between upper-cretaceous biomicrite and natural cements (metamorphic rocks). Therefore, the site of Khushaym Matruk could be a natural analogue for the following waste disposal subsystems:

- cement alteration: observation of fractures in the cement zone,
- impact of temperature on sediments: 3 m thick zone of baked biomicrite,
- interaction between high pH fluids and clay minerals: observation at the vicinity of large fractures crosscutting the biomicrite at some depth, and
- evolution and propagation of a high pH plume in near-field and geosphere matrix.

The present investigation mostly provides qualitative information on possible interaction scenarios. Gaucher et al. /GAU 04/ quote the Khushaym-Matruk analogue in connection with simulations of the diffusion of an alkaline plume in a clay barrier. Limitation in transferability is due to difficulties separating thermal and chemical effects on a large part of the profile. In addition, some clay, particular the baked biomicrite, has been formed in connection with thermal perturbation. These may have strongly hampered further ingress of high pH fluids, but it is not easy to verify. Uncertainties are mainly given by estimation of process age and time duration. For example, duration of episodes with high pH fluid percolation within fracture network is usually not known. In addition, influence of organic matter on high pH fluids may be underestimated.

Localisation and Description

The Khushaym Matruk site (N 31°16’ 570; E 36°14’ 775) is located about 80 km southeast of Amman city (s. Fig. 4.24). The area belongs to the southern extension of Daba Marble Zone /LIN 98/.

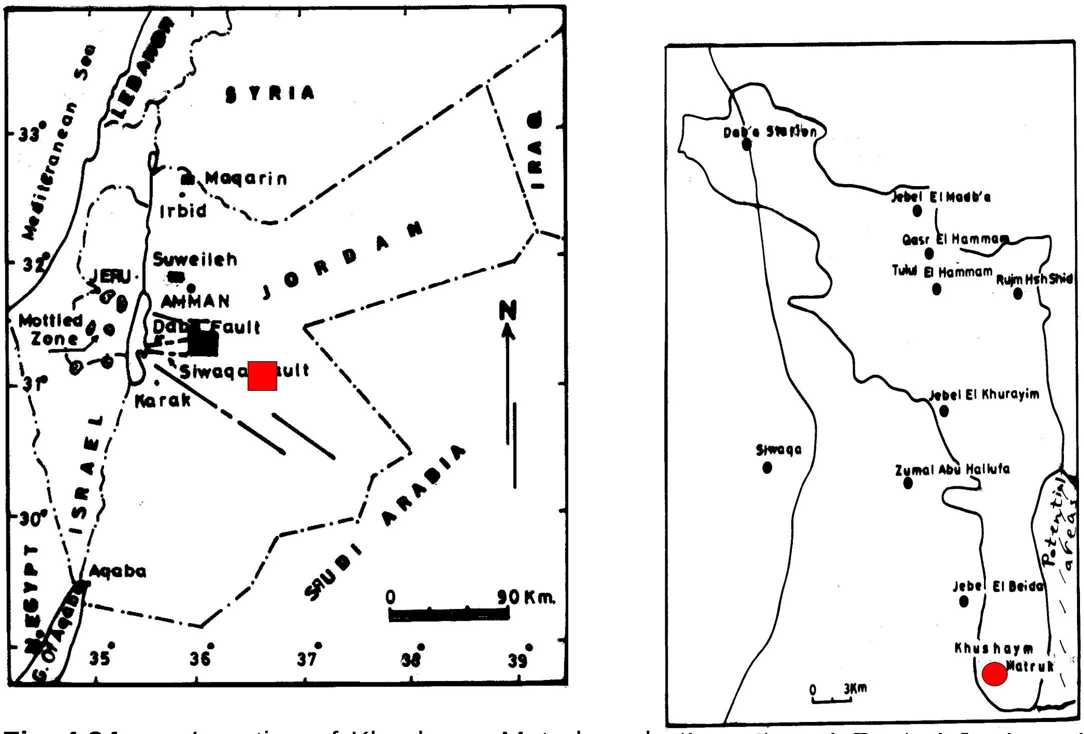


Fig. 4.24 Location of Khushaym Matruk and other sites of Central Jordan where natural cement bodies had been found /PIT 11/

The site itself is located at the western end of a low range of hills. The contact between biomicrite and thermally metamorphosed rocks is clearly visible (Fig. 4.25).

Fig. 4.25 Khushaym Matruk site /PIT 11/

A cap of high temperature grade cement is preserved at the top of the hill. At the basis a grey layer shows the outcrop of the Muwaqqar biomicrite. The discontinuous travertine layer is represented as small ridge above the biomicrite/cement interface.

During Late Cretaceous to Early Eocene time (≈ 90 - ≈ 50 Ma ago) the area was situated in a shallow marine, stable shelf environment of Tethys sea. Due to fluctuations in sea level, transgression took place during Cenomanian times, marine sedimentation until Late Eocene. The following uplift is related to the tectonic movement along Jordan Rift, which is located ≈ 60 km to the west of Siwaqa area and caused gentle folding and faulting. The exposed rocks are thus mainly sedimentary and range in age from Upper Cretaceous (Turonian) to Tertiary (Eocene). Travertines and superficial deposits are Pleistocene to recent age. The travertine deposits are probably linked with episodes of wet climate, during significant alteration of metamorphosed rocks. The general chronological sequence of the lithological units is given in Tab. 4.6.

Tab. 4.6 Lithological units in Central Jordan /PIT 11/

Lithological Units	Age	Thickness (m)
Alluvium and gravel	Holocene – Recent	-
Fluviatile and lacustine gravel	Pleistocene – Recent	-
Travertine	Pleistocene – Recent	-
Um Rijam Chert Limestone Formation (B4)	Eocene	30-80
Muwaqqar Chalk Marl Formation (B3)	Paleocene – Tertiary	70-150
Al-Hisa Phosphorite Formation (B2)	Maestrichtian (Upper Cretaceous)	25-70
Amman Silicified Limestone Formation (B2a)	Campanian	15-80
	(Upper Cretaceous)	
Wadi Umm Ghudran Formation (B1)	Campanian – Santonian	3
Wadi Es – Sir Limestone Formation (A7)	Turonian	30

A discontinuous travertine layer (about 1 to 2 m thick) covers the interface between cement and baked biomicrite at the surface. Green Cr-rich minerals are associated with the travertine. A zone of strongly baked and perturbed biomicrite, about 2.5 to 3 m thick, is located between the cement zone and the apparently unperturbed underlying biomicrite. This baked zone contains both hard and soft micro horizons with different colours, suggesting a transformation of biomicrite by heat and/or chemicals. Information obtained from magnetic investigations and study of organic matter shows, that the layer of baked micrites corresponds to the thermal gradient of the cement zone.

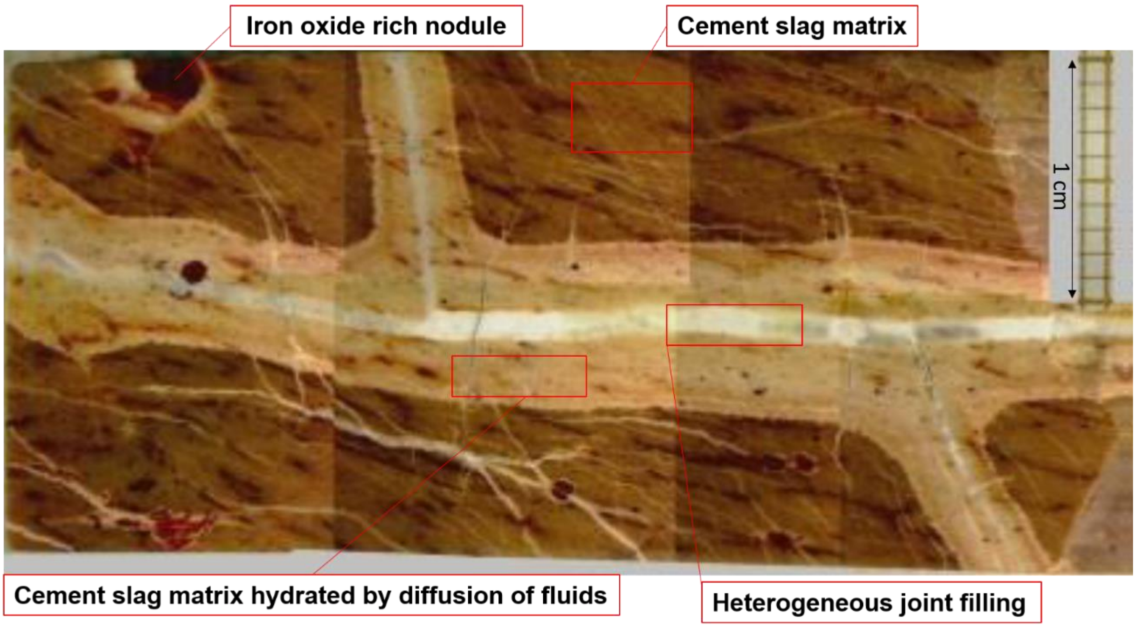
In contrast with Maqarin site, in the biomicrite no pyrite was detected. It is not known whether this is due to surficial rock mass oxidation, pyrite being present at greater depths, or if this is effectively a specificity of the Khushaym Matruk site.

Trench profiles of Khushaym Matruk point out four stratification layers /PIT 11/, TEC 06/:

- a cemented zone at the top with filled fractures (s. Fig. 4.25),
- a Travertin deposit at the basis of the cement body,
- a strongly baked biomicrite, ~ 3 m thick with important textural and chemical transformations as result of high temperature events and pervasive fluid circulation and
- an underlying biomicrite, affected by high pH fluids along large vertical fractures.

Fig. 4.26 Mosaic of several individual pictures of cement sample from Khushaym Matruk /PIT 11/

In the discoloured cement, spurrite has been replaced by CSH and afwillite. Fracture filling is jennite and calcite. Smectitic clay minerals observed in a clay enriched horizon of baked biomicrites



At present day, the groundwater table lies within 150 – 200 m depth. Currently the mean annual precipitation is about 110 mm. Although periods of pluvial climate have been identified in this region during the last 0.5 Ma (personal communication of Prof. Khoury), today the site is totally desaturated.

Investigation

A first sampling of the site was done within the Maqarin Phase IV project (1999 – 2004) in cooperation with Andra, CEA, JNC, Nagra, Nirex, SKB and Jordan University /PIT 13/. The groundwater sampling contains analysis of hyperalkaline springs, as well as other groundwater recharge and discharge zones. Most investigations have focused on a vertical sampling of about 10 m extension across the interface. The sampling was done along a trench that was dug in order to avoid potential surface alteration and weathering effects.

Major outputs

It became obvious, that large vertical fractures, mainly filled with gypsum, crosscut the whole section. Also, the baked zone is perturbed with fractures filled with gypsum or zeolite minerals. Foraminifera tests are often filled with zeolites. Some horizons are enriched of clay minerals (up to 23 wt%). In the baked layer smectitic clay minerals have a lower crystallinity than in the original biomicrite. Quartz and K-feldspar, initially present in the biomicrite, have been replaced by amorphous silica. The clays below the baked zone are more beidellitic nature, with a lower I/S content (60 %) near the baked zone than at depth (80 %). A significant increase in cation exchange capacity is associated with the interface between the baked zone and the less perturbed biomicrite.

The CSH phases seem to be located only within the cement zone, whereas in Maqarin, CSH minerals can be found along distant fractures. This could mean that calcium migration has been hampered, perhaps due to higher clay content in the baked zone.

Interactions between high pH fluids and clay minerals could be studied well along major fractures in baked marls without too much interference. Techer et al. /TEC 04/ have evidenced, that the high pH solutions of the sites sedimentary pile circulated between 110 and 130 ka ago. The age of combustion process is believed to be less than 1 Ma, possibly ~800 ka, considering isotope data obtained on travertine in another Central Jordan site.

Supported FEP

Tab. 4.7 Component FEP:

Buffer/Backfill	
(04) Buffer	x
(05) Backfill	x
Gases, Solutions, Corrosion Products	
(13) Corrosion Products in the repository	x
(14) Repository Solutions	x
Geological Units	
(18) Host Rock	x
Gases and Solutions	
(19) Host Rock Solutions	x

Tab. 4.8 Process FEP:

25	Vertical Movements of earth crust	x
30	Metamorphism	x
41	Corrosion of cement	x
45	Dissolution, Transformation, Neoformation of clay minerals	x
46	Dissolution, Transformation, Neoformation of other minerals	x
47	Chemical Alteration of Organics	x
56	Solution/Gas Flow	x
58	Diffusion	x

References for Khushaym Matruk

/GAU 04/ Gaucher, E., Blanc, P., Matray, J.-M., Michau, N. (2004): Modeling diffusion of an alkaline plume in a clay barrier. Appl. Geochem., 19, 1505-1515.

/LIN 98/ Linklater, C.M. (Ed.): Maqarin phase II report (Nirex S/98/003), 1998.

/PIT 11/ Pitty, A., Alexander, R. (Eds.): A natural analogue study of cement buffered, hyperalkaline groundwaters and their interaction with a repository host rock IV: an examination of the Khushaym Matruk (central Jordan) and Maqarin (northern Jordan) sites. Bedrock Geosciences Technical Report 11-02, 2011.

/TEC 04/ Techer I., Fourcade S., Elie M., Martinez L., Boulvais P., Claude C., Clauer N., Pagel M., Hamelin B. and Lancelot J. (2004) Natural analogue contribution to the understanding of the long-term behaviour of argillaceous formations towards a high-alkaline fluid circulation: study of the Khushaym Matruk site (Central Jordan). Sr, C and O isotopic chemistry, U-Th and K-Ar dating, organic matter characterization. Final Report CNRS-Andra, GdR Forpro G0788, Research Program 2001-VII, 61 p.

/TEC 06/ Techer, I., Khoury, H.N., Salameh, E., Rassineux, F., Claude, C., Clauer, N., Pagel, M., Lancelot, J., Hamelin, B., Jacquot, E., 2005. Propagation of high-alkaline fluids in an argillaceous formation: case study of the Khushaym Matruk natural analogue (Central Jordan). Journal of Geochemical Exploration, 90, (pp.53-67) 2006.

4.4.4.3 Summary and Outlook

The intention of the study was compile analogue studies, which might be useful for supporting aspects of the safety case for a repository of heat generating waste in a clay formation.

Within a first step, the safety goals developed for the safety concept of a potential German repository in a clay formation and the materials foreseen to be used in the respective repository concept have been documented. On that basis, a number of analogue studies related to clay have been compiled in the second step and evaluated with regard to their contribution to either the safety goals or to the behaviour of materials intended to be used in the repository. Currently the document contains 29 analogue studies. The studies are included in short form. Detailed information can be referred to from the reference literature. It became obvious that the wide spread of external impacts on materials mentioned within analogues (and which will be also found within the repository) and their long residence time would be very useful within the assessment of long-term behaviour of repository materials and host rocks.

Within a third step analogue information had been related to the process and component FEP derived for a potential German repository in clay. If there might be a benefit for a FEP, it had been marked within a table on the end of each analogues documentation. In addition, an excel table had been performed with these information for the purpose of searching and analysis functions. The table contains up to now about 200 data entries.

Therefore, a basis for documentation of analogues useful for safety concepts of heat generating waste in clay formation had been established. The data management in table form offers a possibility of several analysis tools like e. g. searching functions. Hence analogues, which might contain information about special safety functions or FEP can be easily found. On the other site absent information for safety functions and FEP become obvious.

Until now a statement about the data quality and their benefit in performance assessment is not implemented. In addition, data for parameter are not deposited within the table, just the information that they are available. Here, further work is recommended to evaluate the available information and compile it in an improved. database.

5 Summary and conclusions

The work performed within this project contributed to different aspects of the safety case, namely the assessment basis, methods and strategies, long-term safety assessment and additional lines of evidence to be used in a safety case. Current national and international developments have been followed and discussed, R&D projects with relevance for post-closure safety of radioactive waste repositories have been analysed and evaluated to improve process understanding and, where possible, new conceptual models and/or parameter sets to be considered in performance assessment have been proposed.

Developments in other countries and at the international level in general have been followed by participation in international committees and working groups, like RWMC, IGSC, Clay Club, Salt Club, Crystalline Club and IAEA activities regarding the biosphere. GRS was deeply involved in working groups and topical sessions to evaluate and further develop the status of safety relevant issues related to the safety case of a deep geological repository (DGR). IGSC topical sessions on (i) the relevance of gases in the safety case, (ii) the role and use of geoscientific arguments in the siting process, and (iii) criticality and safeguards in a DGR were organised, evaluated and summarized. These topical sessions reflect the current state of each topic in the NEA member countries and therewith represents a broad range of international experiences. This pool of knowledge can be used to gain increased insight in specific aspects of the safety case and to check against the national approaches and may initiate new R&D work.

Aspects related to the communication of the safety case are currently one key issue considered by working groups of the NEA. Two activities are highlighted in this report, communication of complex technical contents of the safety case to lay people and how to transfer records, knowledge and memories of a radioactive waste repository after its closure to future generations. The first activity has been performed by a working group of the IGSC, who was mandated to investigate the issue of communicating scientific information with non-technical stakeholders. Based on a review of projects, initiatives and local communication activities with public stakeholders, effective communication approaches/strategies were synthesized. Difficulties and challenges of the communication have been documented and ideas for improving communication were presented.

The latter aspect has been addressed in the NEA Initiative on the Preservation of Records, Knowledge and Memory (RK&M) Across Generations. Geological repositories are designed to be intrinsically safe and do not rely on human maintenance or intervention. Nevertheless, there is no intention to abandon these repositories or to lose oversight over them. This means records, knowledge and memory of the repository should be preserved as long as possible and therewith contribute to avoiding inadvertent human intrusion and supporting informed decision making in the future. During the project a systemic strategy consisting of a menu of mechanisms and approaches that can be used to preserve RK&M across generations has been developed. Particularly support was given for the development of a strategy to create a Set of Essential Records, which can be understood as a collection of the most important records for waste disposal selected for permanent preservation during the repository lifetime. It provides sufficient information for current and future generations to ensure an adequate understanding of the repository system and its performance enabling them to review and verify the repository performance and the safety case to assist in making informed decisions based on an assessment of the consequences.

The assessment of the post-closure radiological consequences forms the core of the safety case for a radioactive waste disposal facility. This involves a comprehensive approach for the handling of the uncertainties, especially the analysis of the possible evolutions of the repository system (scenarios) and the resulting potential radiological consequences. According to international best practice, the development of scenarios for safety assessments of deep geological repositories is based on FEP. With regard to this the NEA Salt Club started an activity for developing an international FEP database for repositories in salt. The developed SaltFEP data base is available on an internet platform and can provide future scenario developers with information about relevant processes and effects in all compartments of a repository system including a comprehensive reference data base denoted as Salt Knowledge Archive.

During the last decade significant work on national and international level has been performed with respect to the process of scenario development and analysis for the disposal of radioactive waste and the strategies have changed. GRS contributed to a survey and a workshop organized by the NEA working group IGSC to evaluate the experience acquired in developing scenarios and managing uncertainties in IGSC member countries. Key issues are discussed in this report. Efforts have been made to ensure comprehensiveness, traceability of decisions, and the integration and logical structuring of interdisciplinary knowledge in the development of scenarios. Scenarios and scenario development are now more prominently featured in the documentation of safety cases than in the past, with an emphasis on transparency and traceability of decisions. The potential for further development is still seen in communicating the role and choice of scenarios to wider audiences and in the issue of assigning probabilities to FEP and scenarios. Especially the treatment of improbable scenarios is a topic currently addressed by the German scenario working group. Improbable scenarios include evolutions with a residual probability of occurrence below 1 %, and these have to be analysed and evaluated. It is consensus of the Working Group that it is reasonable to consider only scenarios that have at least a residual probability of occurrence. Unrealistic with a zero or almost zero probability scenarios should be excluded. Instead it is useful to use "What if scenarios" to test the robustness of the repository system.

In the general treatment of uncertainties of a safety case, besides the uncertainties about the future evolution of the repository system, uncertainties about the actual values of model parameters are of high relevance. Such uncertainties can be addressed directly in safety assessment calculations via deterministic and/or probabilistic approaches. Probabilistic uncertainty and sensitivity analysis is considered an essential tool for analysing numerical models for repository performance assessment. Specifically, sensitivity analysis can yield valuable information about the model behaviour and help improving system understanding. During PAMINA and afterwards the methodological approaches and numerical tools for sensitivity analysis have been significantly further developed. As part of this project a collaboration with groups from USA, Belgium and Finland was initiated to compare the approaches for probabilistic uncertainty and sensitivity analysis and to learn from each other. Several comparison cases, based on the national programmes, were selected for investigation. So far only orienting calculation results from SANDIA and GRS are available. They show that the tools DAKOTA and RepoSUN calculate very similar rank correlation coefficients, which can be seen as a mutual verification of the tools. Even on the small basis of 50 model runs these tools seem to identify the leading sensitivities of the SNL shale repository model; this, however, needs further confirmation, based on a higher sample size. In addition, further investigations and comparisons are foreseen including the work of the groups from Finland and Belgium. Finally, conclusions should be drawn on the significance of different methods, sample sizes necessary for reliable sensitivity analysis, influence of model complexity and on the interpretation of sensitivity analysis in the context of different repository systems.

Concerning radionuclide mobility in cooperation with NAGRA a method for deriving the average and nominal maximum radionuclide inventories of vitrified waste produced at La Hague was developed and applied. For safety assessment studies, the implemented method is considered to be an acceptable approach. However, for the future it is considered worthwhile to examine a larger variety of glasses to build up a data base of possible inventories at an international level; this will allow cross-checks as well as an assessment of the accuracy of the inventory data.

Major work was devoted for participation in the CAST project (CArbon-14 Source Term), which aimed to develop understanding of the potential release mechanisms of ^{14}C from radioactive waste materials under conditions relevant to waste packaging and disposal to underground geological disposal facilities. GRS participated in a work package with the aim to consider the results produced in the experimental work packages at the scale of their repository system and to analyse their impact in terms of long-term safety. For this issue, the preliminary safety assessment for Gorleben was taken as basis and only release from Zircaloys and steel was regarded. The calculations show that the consequences of the ^{14}C release from the waste in the early phase of the repository, determined by the radiological safety indicator (RGI), are to a large part controlled by the quantity of the ^{14}C released. The temporal behaviour of the ^{14}C release only shows a minor impact on the RGI indicator. The potential to reduce the conservatism in the assumption of the amount of ^{14}C during the early phase of the repository is high according to the results obtained in the First Nuclides and the CAST projects. The first experimental results from CAST suggest values for the fraction, which is instantaneously released, in the range of 1 %, i. e. at the lower boundary of the range used in the parameter variations and also much lower than assumed in the VSG reference scenario.

In the frame of the TDB project of OECD/NEA a state of the art report on the topic high ionic strength solutions – “State of the art report to assess modelling and experimental approaches" is currently created. The report illustrates to which extent geochemical processes in high mineralised solutions can be modelled by the Pitzer approach. The German contribution to this report comprised the analysis of the status of iron and lead. The analysis of available data for ferrous iron showed that data sets, particularly for the system $FeCl_2$ - Na, K, Mg, Ca - H_2O are available to derive a Pitzer model, whereas for the $FeSO_4$ system relevant data are lacking. In order to derive a Pitzer model for ferric iron data are lacking and further experiments like spectroscopic measurements for quantification of relevant complexes are needed. It is recommended to restrict such experiments and the model to the conditions relevant for a repository.

With respect to microbial effects further review work was performed for repositories in clay and salt rock. With respect to a deep geological repository for heat generating waste in a clay rock the work aimed at obtaining a quantitative estimation of the maximum possible effect of microbial processes. It resulted in a conclusion that such estimation does require the application of a dedicated software tool because of the far too complex system of competing or synergistic microbial subpopulations interacting with different repository components. These interactions are not only distributed over the whole repository space but also develop within a timescale of years, possibly proceeding for several thousand years, and are influenced by the evolutions of temperature, pore space and nutrient concentrations within the repository system. To account for these evolutions, the population dynamics of microbial community and its interactions with the repository components within a reasonable working effort, a use of an on-the-shelf software tool would be a preferable option. For salt rock GRS has contributed to the report on the microbial processes relevant for nuclear waste repositories in salt rock produced in the frame of the Salt Club. The report summarizes the potential role of microorganisms in nuclear waste repositories in rock salt using available information on the microbial ecology of hypersaline environments, the bioenergetics of survival under high ionic strength conditions, and “repository microbiology” related studies. GRS contributions specifically concerned the consideration of the probable pressure effect on the vitality and activity of the exogenous microorganisms, on the possible microbial metabolic pathways, and on cellulose degradation at the repository conditions.

A significant part of the project was dedicated to the investigation and use of analogues in safety cases. Firstly, a workshop was organised to discuss the potential for natural and anthropogenic analogue studies to contribute to safety cases for radioactive waste repositories in salt formations. Presentations were given on many analogue sites and systems from different countries. Discussions at the workshop addressed aspects that are particularly relevant to the safety concept for radioactive waste disposal in salt: (1) the long-term integrity of rock salt formations, (2) the integrity of technical barriers, and (3) microbial, chemical and transport processes. A diverse range of natural systems were discussed as potential analogues for the integrity of rock salt. These included the deformation of anhydrite layers in rock salt; the response of rock salt to mechanical and thermal loads; and the isotopic signatures of syngenetic waters contained in fluid inclusions. Some anthropogenic examples drawn from the oil and gas industries, and from hazardous waste disposal, were proposed as analogues for the integrity of (geo)technical barriers. Studies on natural and anthropogenic salt-brine systems were identified as potential analogues for the radionuclide sorption and (co)precipitation process that may take place in the repository near and far fields, as well as for understanding the significance of hydrocarbons and microbial processes. It was evident from discussions at the workshop that there are some specific technical issues that may benefit from further analogue study, particularly the compaction of crushed salt backfill, the viability of microbes in the near-field, the stability of plugs and seals, the deformation of anhydrite, and isotope signatures in fluid inclusions.

Moreover, after finalisation of the investigations at the Ruprechtov site in Czech Republic a wrap-up of the natural analogue study has been performed. The resulting status report provides a brief overview on the different roles of analogues in national repository programmes and the evolution of analogue application in safety cases. It compiles and critically discusses the decisions regarding the selection of the Ruprechtov site as a natural analogue, classifies the site with regard to the type of uranium accumulation and displays the iterative steps, decisions and evolution of knowledge during the investigation of the site. Advantages and disadvantages of the stepwise approach are discussed. Further, the report describes the experiences obtained, particularly in the selection and application of experimental laboratory and field methods, and outlines the scheme, by which these methods have contributed to understanding and characterizing the main features of the site. Finally, the main findings relevant for a safety case for a radioactive waste repository were illustrated, the lessons learned compiled and from that recommendations for future R&D were given.

A third task was devoted to the compilation of analogue studies for radioactive waste repositories in clay formations and a systematic analysis, how such studies can support a safety case. This task was based on the German safety concept and assessment strategy for a repository with heat-generating radioactive waste, which was developed during the project ANSICHT. According to the safety concept, the containment of the radioactive waste is primarily achieved by hindering the radionuclide transport by chemical and physical processes resulting from positive properties of the clay host rock in combination with geotechnical barriers. This primary goal is achieved by a set of sub-goals listed in the safety concept. A selected number of existing analogue studies were then reviewed with regard to their contribution to one or more of these safety goals. Furthermore, for comprehensiveness of materials and processes expected to occur in the repository, the FEP catalogue was used and for each analogue it was checked, to which of the FEP the respective analogue study contributes. The work showed that for several FEP a number of analogues exist and for some FEP no analogues were found. Based on this evaluation more analogue studies should be evaluated particularly to identify (potential) analogues for those FEP, where analogues are missing.

With regard to bentonite re-saturation an aspect was addressed, which has not been in the focus of research so far, namely the water uptake under a limited water supply rate from the rock, which might reflect the conditions in a repository system. So far bentonite saturation experiments have typically been performed with unimpeded access to water. In this project an experimental set-up was developed and optimized, where water flow rates where adjusted, which are below the uptake rates of the bentonite samples. Therewith, time dependent data for water uptake under restricted water supply conditions could be derived. The transport code VIPER was further developed in order to simulate the limited water uptake. The updated version of the code was then able to simulate the water uptake in the experiments fairly well. One important observation of the experiments was that a fully saturated zone in the bentonite sample, which is always formed in experiments with unlimited water uptake, does not form in early stages of the experiment but is built only at later points in time.

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