National and International Networking for Research and Competence Maintenance of the Safety Case

GRS - 858

Sachbericht zum Verwendungsnachweis

Verbundprojekt

Flankierende nationale und internationale Vernetzung der GRS für Forschung und Kompetenzerhalt

FLANKE

in der Fördermaßnahme

BMUKN-Forschungsförderung zur nuklearen Sicherheit

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Projektlaufzeit: 01.10.2024 –31.12.2025

Erstellungsdatum: 30.06.2026

Projektpartner

Förderkennzeichen 02E12184

Dieses Forschungs- und Entwicklungsprojekt wurde durch das Bundesministerium für Umwelt, Klimaschutz, Naturschutz und nukleare Sicherheit gefördert und vom Projektträger Karlsruhe (PTKA) betreut. Die Verantwortung für den Inhalt dieser Veröffentlichung liegt bei den Autorinnen und Autoren.

Gefördert durch:

Bundesministerium
für Umwelt, Klimaschutz, Naturschutz
und nukleare Sicherheit

Gesellschaft für Anlagen-
und Reaktorsicherheit
(GRS) gGmbH

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Remark:

This report refers to the in-house research project 02E12184 which has been funded by German Federal Ministry for the Environment, Climate Action, Nature Conservation and Nuclear Safety (BMUKN).

The work was conducted by Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) gGmbH.

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GRS - 858
ISBN 978-3-911727-51-8

Keywords

Clay, Crystalline rock, Knowledge management, Modelling, Permafrost, Radioactive waste, Rock salt, Safety Assessment, Safety Case, Sensitivity analysis, Uncertainty

Kurzzusammenfassung

Das Vorhaben "Flankierende nationale und internationale Vernetzung der GRS für Forschung und Kompetenzerhalt (FLANKE)" dient zur Verfolgung des internationalen Stands des Wissens zu allen Aspekten eines Safety Case für Endlager. Durch die Mitarbeit in internationalen Gremien und Arbeitsgruppen wird gewährleistet, dass die verwendeten Methoden, Ansätze und Rechenprogramme eines Safety Case in Deutschland dem internationalen Stand von Wissenschaft und Technik entsprechen.

Im Einzelnen wurden im Vorhaben FLANKE Ergebnisse zu verschiedenen Themen erzielt. Die aktuellen Projekte der OECD NEA sowie das Safety Case Symposium haben neue Entwicklungen zum Safety Case aufgezeigt, insbesondere wie sich der Safety Case während des Endlagerprogramms entwickelt, und dass in vielen Ländern Systeme zum Management von Anforderungen immer wichtiger werden. Zum Wissenstransfer und Kompetenzerhalt beim Safety Case wurden auf internationaler Ebene u.a. das Next Generation Network (NGN) der IGSC gegründet und etabliert. Die Leistungsfähigkeit sowie die Stärken und Schwächen verschiedener Methoden der Sensitivitätsanalyse wurden anhand eines internationalen Benchmarks an ausgewählten Modellrechnungen zu verschiedenen Endlagern untersucht und herausgearbeitet. Im Hinblick auf Modellrechnungen wurden neue Methoden zur Erstellung von Kluftnetzwerken für Strömungsmodelle erfolgreich getestet und anhand von Experimenten das Verständnis über Gefrierprozesse in Klüften und die Bedeutung der räumlich heterogenen Gefrierprozesse für die Entwicklung der Wasserdurchlässigkeit bei Permafrostbedingungen deutlich verbessert.

Die genannten Ergebnisse werden bei GRS direkt zur Aktualisierung von Methoden, Parametern und Rechenprogrammen für den Sicherheitsnachweis verwendet. Die Rückspiegelung der Ergebnisse an andere deutsche Institutionen wie z.B. die Bundesgesellschaft für Endlagerung mbH (BGE) oder das Bundesamt für die sichere Entsorgung (BASE) ermöglicht auch ihnen die Nutzung der Ergebnisse, z.B. zur Verbesserung ihrer Rechenprogramme für die Sicherheitsnachweise der vorhandenen Endlager aber auch für die kommenden Schritte der Standortauswahl.

Zusammenfassung

Die im internationalen Rahmen etablierte Methodik der Sicherheitsbewertung für geologische Endlager, der Safety Case, wird seit mehr als zwanzig Jahren angewandt und insbesondere in Gremien der Nuclear Energy Agency (NEA) und der International Atomic Energy Agency (IAEA) stetig weiterentwickelt. Diese allgemeine Vorgehensweise bei einer Sicherheitsbewertung muss mit den nationalen Regelwerken übereinstimmen, sie sollte aber auch international akzeptiert sein und ist daher fortlaufend an die internationalen Entwicklungen wie auch an die neuen Erkenntnisse aus Forschung, Wissenschaft und Technik anzupassen. Das Projekt hat dazu beigetragen, das Verständnis für einen Safety Case zu vertiefen, neue Erkenntnisse aus internationalen Forschungsarbeiten für den nationalen Sicherheitsnachweis auszuwerten und die Methodik für Langzeitsicherheitsbewertungen entsprechend dem Stand der Technik weiterzuentwickeln.

Eine wichtige Aufgabe des Projekts ist die Mitarbeit in internationalen Gremien und Arbeitsgruppen, um neue Entwicklungen in anderen Ländern und auf internationaler Ebene zu verfolgen und zur Entwicklung von Strategien, Methoden und Werkzeugen für einen Sicherheitsnachweis geologischer Tiefenlager beizutragen. Eine aktive Teilnahme erfolgte zum einen in Arbeitsgruppen der OECD-NEA, namentlich der Integration Group for the Safety Case (IGSC), der Arbeitsgruppe Information, Data and Knowledge Management (WP-IDKM) und zugehörigen Expertengruppen, dem Salt Club, Clay Club sowie dem Crystalline Club. Zum anderen spielte die Teilnahme in den internationalen Arbeitsgruppen und Projekten Joint Sensitivity Analysis Exercise (JOSA), Task Force on Engineered Barriers (EBS), CatchNet und DECOVALEX-2027 eine wichtige Rolle.

Ein Schwerpunkt der Arbeiten der IGSC während der Laufzeit dieses Vorhabens waren die erfolgreiche Durchführung, die Auswertung und die Veröffentlichung der Proceedings des Safety Case Symposiums 2024 in Budapest. Initiiert durch ihre Gründung und aktive Mitarbeit auf dem Symposium hat sich in der IGSC jetzt das Next Generation Network (NGN) etabliert und bildet seit Oktober 2025 formal eine Adhoc-Gruppe der IGSC. Übergeordneten Ziele der NGN sind es, die berufliche Weiterentwicklung zu fördern, neue Stimmen in die Community zu integrieren, einen strukturierten Wissenstransfer zu fördern sowie vielfältige berufliche Netzwerke aufzubauen. Mitglieder des NGN arbeiten jetzt auch vermehrt in weiteren Aktivitäten der IGSC mit. Schließlich wurden die Arbeiten im IGSC-GeneSiS-Projekt weitergeführt, wo Erfahrungen aus der Erstellung von Sicherheitsnachweisen beginnend mit generischen Phasen hin zu standortspezifischen

Phasen zusammengestellt werden und Ländern, die sich in frühen Phasen des Endlagerprogramms befinden, als Anleitung bzw. Hilfestellung dienen sollen. Hier liegen die Abschlussberichte zum Vorhaben mittlerweile im Entwurf vor und werden in 2026 vor der Veröffentlichung von den Gremien und Arbeitsgruppen der NEA geprüft.

Im Salt Club der NEA war GRS hauptsächlich an den Arbeiten für die NEA Salt Club Arbeitsgruppe “The role of scenarios in the modelling strategy for the safety assessment for deep geological repositories” beteiligt. Diese Arbeitsgruppe befasst sich aktuell mit der Untersuchung von Möglichkeiten für die Abbildung von Szenarien auf numerische Modelle (bzw. umgekehrt). Die Gesamtheit von ausgewählten Szenarien deckt die Unsicherheiten der zukünftigen Entwicklung eines Endlagersystems ab; es ist jedoch noch unklar, wie der Szenarienansatz mit der Modellierungsstrategie verknüpft ist. Empfehlungen zum Umgang mit Szenarienunsicherheiten im Rahmen der Modellierungsstrategie für Zeiträume von bis zu einer Million Jahren existieren nicht. Die Arbeiten des Salt Clubs zu diesem Thema sollen im Rahmen einer Analyse nationaler Programme für Endlager in Salzformationen erfolgen. Zum Auftakt wurde dafür ein Fragebogen entwickelt, der dazu dient, Erfahrungen und Möglichkeiten hinsichtlich der Verknüpfung zwischen Szenarien und der Modellierungsstrategie zu erfassen.

Der NEA Clay Club erzielte wichtige Fortschritte im Verständnis tonreicher Gesteine als Wirtsgesteine für die Endlagerung radioaktiver Abfälle. 2024 waren ein Workshop zur Porenwasserchemie und ein Projekt zu Druckanomalien im Fokus. Die Untersuchungen zu Druckanomalien zeigen, dass in Tonformationen meist Unterdruck herrscht, bedingt durch geologische Prozesse wie Erosion. Neue Modelle verbessern die Auswertung von Messdaten und betonen die Bedeutung langfristiger Überwachung. Insgesamt bestätigen die Ergebnisse die Eignung von Tonformationen als sichere Barrieren, weisen aber zugleich auf die Notwendigkeit standortspezifischer und detaillierter Analysen hin. Die Veröffentlichung des CLAYWAT-Projekts in 2025 beschreibt umfassend die neuen Erkenntnisse zum Verhalten von Wasser in Nanoporen.

Der NEA Crystalline Club fördert den internationalen Austausch zum Verständnis kristalliner Gesteine als Wirtsgesteine für die Endlagerung hochradioaktiver Abfälle. Im Zeitraum 2024–2025 standen in seiner Arbeit die beiden Themen (i) chemische Bedingungen die relevant für das Verhalten eines Endlagers im kristallinen Gestein sind und insbesondere deren Einfluss auf die Korrosion von Endlagerbehältern, sowie (ii) die Prüfung der Machbarkeit eines Katalogs von Eigenschaften (Catalogue of Characteristics) kristalliner Gesteine im Vordergrund. Ein zentrales Ergebnis war der Aufbau einer umfangreichen Literaturdatenbank (Cryschem) mit über 600 Einträgen, die in 2026 veröffentlicht werden soll. Ob ein Catalogue of Characteristics inklusive einer Analyse von Erfahrungen, Herausforderungen und einer möglichen Roadmap einzelner Länder realisierbar ist, wird derzeit noch diskutiert.

Radioaktive Abfälle entstehen aus einer Vielzahl unterschiedlicher Quellen, die den gesamten Kernbrennstoffkreislauf sowie diverse Anwendungsbereiche in Industrie, Medizin, Verteidigung und Forschung umfassen. Diese Abfälle müssen langzeitig entsorgt werden. Die Zeiträume von Endlagerprogrammen für radioaktiver Abfälle von ihrer Initiierung bis zum Verschluss des Endlagers umfassen typischerweise viele Dekaden. Diese Zeiträume bringen komplexe Herausforderungen mit sich, die sich über mehrere Generationen von Fachkräften sowie über verschiedene technologische Entwicklungsstufen erstrecken. Während des Endlagerprogramms wird ein umfangreiches Volumen an Daten und Informationen generiert. Angesichts der Herausforderungen bei der Verwaltung dieser kritischen Informationen prüfen viele Länder derzeit die Entwicklung eines „digitalen Sicherheitsnachweises", eines innovativen Ansatzes zur umfassenden Nachverfolgung und Dokumentation der Prozesse im Bereich der Entsorgung radioaktiver Abfälle. Zudem beginnen viele Länder damit aus der Fülle an Daten und Informationen eine Auswahl und Zusammenstellung eines strukturierten Satzes an essentiellen Unterlagen (Set of Essential Records, SER) zu erstellen. Damit soll sichergestellt werden, dass künftige Entscheidungsträger die mit radioaktiven Abfällen verbundenen Gefahren über deren gesamten Lebenszyklus hinweg wirksam beherrschen können. Darüber hinaus gibt es mehr und mehr gemeinsame Bestrebungen bei der Entwicklung von Strategien, die das Wissen um Endlager für radioaktive Abfälle auch über extrem lange Zeiträume hinweg bewahren. Die genannten Aspekte werden international insbesondere von der NEA-Arbeitsgruppe „Information, Data and Knowledge Management (WP-IDKM) adressiert und wurden 2025 auf dem Symposium in Yokohama vorgestellt mit der internationalen Gemeinschaft diskutiert. Ein weiterer Aspekt der derzeitigen Arbeiten ist die Frage inwieweit moderne Technologien, wie künstliche Intelligenz zu diesen Themen, beispielsweise der Auswahl und Zusammenstellung essentieller Unterlagen beitragen können.

Die Joint Sensitivity Analysis Group (JOSA) wurde vor sieben Jahren ins Leben gerufen. Der Schwerpunkt der Arbeiten in JOSA liegt auf der Verwendung von Sensitivitätsanalysen (SA) ausgewählter Rechenfäll mit dem übergeordneten Ziel, Leitlinien für die Durchführung solcher Analysen im Rahmen von Sicherheitsbewertungen für geologische Endlager zu entwickeln und bereitzustellen. Das Ziel der Arbeiten besteht darin, ein besseres Verständnis der Stärken und Schwächen verschiedener SA-Methoden zu erlangen, die Leistungsfähigkeit der Methoden zu bestimmen und Best Practices und andere aus dem Benchmark gewonnene Erkenntnisse herauszuarbeiten. Im Jahr 2025 hat die Phase 3 von JOSA begonnen. Als eines der Themen, die in der dritten Phase aufgegriffen wurden, konzentrierte sich die Arbeit des GRS auf die Untersuchung von Screening-Methoden – speziell auf die Morris-Screening-Methode. Diese Methode untersucht die Sensitivität von Parametern basierend auf den Auswirkungen, die kleine lokale Änderungen einzelner Parameter auf das Modellergebnis haben. Die Ergebnisse der GRS-Modellrechnungen für ein Endlager mit schwach- und mittelradioaktiven Abfällen deuten darauf hin, dass für einen komplexen Fall große Stichprobenumfänge mit mindestens 1000 Trajektorien und gut strukturierte Morris-Stichproben erforderlich sind, um Ausreißer und Unregelmäßigkeiten in den Ergebnissen der Morris-Sensitivitätsmaße zu minimieren, die es erheblich erschweren, Parameter als sehr wichtig, weniger wichtig oder (nahezu) unwichtig einzustufen. Der LILW-Fall zeigt ein komplexes Verhalten – einschließlich quasi-diskreter Verhaltensweisen –, das zu sprunghaften Veränderungen der Modell-Ausgabewerte führen kann. Die Morris-Methode scheint geeignet zu sein, alle potenziell wichtigen Parameter und Wechselwirkungen mit einer relativ geringen Anzahl von Durchläufen zu identifizieren. Die Morris-Methode eignet sich nicht dazu, sämtliche Signifikanzgrade der verschiedenen Parameter und Wechselwirkungen zu klassifizieren, da sie als Screening-Verfahren konzipiert wurde und nicht als quantifizierende Methode, wie etwa die varianzbasierte Sensitivitätsanalyse. Letztlich besteht ein großer Vorteil der Morris-Methode darin, die Anzahl der Parameter für weiterführende, eingehende Analysen, beispielsweise mittels varianzbasierter oder anderer Verfahren, reduzieren zu können.

Im Rahmen des von der GRS geleiteten Benchmark 14a der Task Force EBS wurde systematisch untersucht, wie gut verschiedene Modellierungsansätze das hydraulische Verhalten von verdichtetem MX-80-Bentonit bei begrenzter Wasserzufuhr abbilden können. Eine Reihe von Laborexperimenten, die von der GRS im Projekt WiGru-7 /NOS 18/ durchgeführt wurden, lieferte hierfür einen wertvollen Referenzdatensatz. Der Vergleich numerischer Simulationen mit den zugrundeliegenden experimentellen Beobachtungen zeigt, dass die angewandten Modellierungsansätze – insbesondere die COMSOL-VIPER-Schnittstelle – grundsätzlich in der Lage sind, die wesentlichen Merkmale der Bentonit-Hydratation zu erfassen. Dies bestätigt zudem die Eignung der kürzlich in die COMSOL-VIPER-Schnittstelle implementierten Neumann-Randbedingung für die

Darstellung von Bedingungen mit begrenztem Zufluss. Der Vergleich deckte jedoch auch erhebliche Ungewissheiten hinsichtlich der experimentellen Randbedingungen auf, insbesondere bezüglich der Genauigkeit der Spritzenpumpe bei sehr geringen Flussraten. Tests zur Pumpenleistung belegten, dass die tatsächlichen Flussraten erheblich von den Nennwerten abweichen konnten. Diese Erkenntnis erklärt die zunächst festgestellten Diskrepanzen zwischen Modellierungsergebnissen und experimentellen Daten und unterstreicht, wie wichtig eine sorgfältige Überprüfung der Randbedingungen bei derartigen Experimenten ist. Durch die Verwendung effektiver, aus gravimetrischen Messungen abgeleiteter Zuflussraten wurde eine konsistente Grundlage für den Modellvergleich geschaffen. Dieser Ansatz ermöglicht einen aussagekräftigeren Vergleich sowohl zwischen Modellierungs- und Experimentalergebnissen als auch zwischen den beteiligten Teams. Derzeit wird ein abschließender quantitativer Vergleich vorbereitet, der als Grundlage für eine gemeinsame Publikation dienen soll.

Ergänzende experimentelle Arbeiten in CatchNet unter Verwendung von 3D-gedruckten Bruchmodellen lieferten neue qualitative Erkenntnisse über Gefrierprozesse in Klüften. Die Beobachtungen zeigen, dass die Eisbildung in einer Kluft in mehreren Phasen erfolgt: Zunächst bildet sich ein Eis-Film entlang der Bruchflächen, gefolgt von einer langsameren Ausbreitung lokaler Gefrierfronten. Wichtig ist, dass die hydraulische Konnektivität in frühen Gefrierphasen erhalten bleiben kann, was auf ein komplexes Zusammenspiel zwischen Phasenübergang und Strömungsprozessen hindeutet. Die Ergebnisse verdeutlichen den ungleichmäßigen und transienten Charakter von Phasenübergängen in Klüften und unterstreichen die Bedeutung der räumlich heterogenen Gefrierprozesse für die Beurteilung der Permeabilitätsentwicklung in Klüften unter Gefrierbedingungen.

Ein Teil des DECOVALEX-Projekts konzentriert sich auf den systematischen Vergleich von Modellen und Methoden, die für die Langzeitsicherheitsanalyse (PA) von Endlagern für radioaktive Abfälle eingesetzt werden. Innerhalb dieses Vergleichs werden zwei parallele, wirtgesteinsspezifische Aktivitäten verfolgt – namentlich die „PA Salt Task“ und die „PA Crystalline Task“ –, die sich jeweils mit der Sicherheitsbewertung von Endlagern in Salz- bzw. kristallinen Formationen befassen. In diesem Bericht wurden die vom Projekt unterstützten Arbeiten für Endlager in Salzformationen betrachtet. In der jetzigen Projektphase begannen die teilnehmenden Modellierungsteams mit der Implementierung einer Reihe von Benchmark-Fällen, die jeweils separat diffusionsdominierte Transportprozesse sowie das Kriechverhalten von Salz adressieren. Die bisherigen

Ergebnisse des Benchmarks zeigen, dass hinsichtlich der analytischen Lösung des Diffusions-Benchmarks eine sehr gute Übereinstimmung zwischen den teilnehmenden Teams erreicht wurde. Beim Kriech-Benchmark traten lediglich geringfügige Abweichungen auf. Diese Abweichungen lassen sich durch Unterschiede in den zugrundeliegenden Berechnungsansätzen erklären; eine Anpassung der analytischen Lösung behebt dieses Problem erfolgreich. In den nächsten Schritten der Studie werden für die betrachteten Benchmarks Unsicherheits- und Sensitivitätsanalysen durchgeführt. Darüber hinaus werden Unsicherheits- und Sensitivitätsanalysen für einen erweiterten Referenzfall vorgenommen, der aus DECOVALEX-2023 abgeleitet wurde.

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1 Introduction

The overarching objective of this project is to monitor the international state of knowledge regarding all aspects of the safety case within international bodies and working groups. This aims to ensure that methods, approaches, and computational tools are continuously advanced to align with international standards. Concurrently, specific approaches and experiences developed within the German repository program are to be introduced into these international working groups, thereby contributing to the further development of these methods, approaches, and computational tools.

This objective is achieved by active participation, in working groups of the OECD-NEA, namely the Integration Group for the Safety Case (IGSC), the Working Party on Information, Data and Knowledge Management (WP-IDKM), and associated expert groups as well as the Salt Club, Clay Club, and Crystalline Club. In addition, participation in the international working groups and projects Joint Sensitivity Analysis Exercise (JOSA), Task Force on Engineered Barriers (EBS), CatchNet, and DECOVALEX-2027 play an important role.

The IGSC is continuously further developing strategies and methods for the safety case that supports decision making at each stage of repository development. It presents underlying evidence and methods that give confidence in the quality of scientific and institutional processes, as well as in the results of analyses. Current key activities of the IGSC have been the planning and implementation of the Safety Case Symposium in Budapest and now the finalisation of the GeneSiS project (From generic to site-specific safety cases). The Next generation network, formed in advance of the symposium, has been well established and is now participating in different activities of IGSC. To help accomplish its activities, the IGSC is supported by subgroups carrying out tasks on specific topics. Three subgroups focus on the feasibility of repositories in three different generic host rock types: Clay Club, Salt Club and Crystalline Club.

The objective of the Salt Club is to generate and exchange scientific information regarding rock salt as a host rock for deep geological repositories for high-level radioactive waste. In addition to technical and scientific aspects, the Salt Club also aims to foster the education and professional development of future experts in the field of rock salt. Currently the salt club has started an activity with to investigate possibilities for mapping scenarios to the numerical models (or vice versa) by investigating national programs for repositories in salt.

The goal of the Clay Club is to develop and exchange scientific information on clay host rock for deep geological repositories for high-level radioactive waste between the member countries. The Clay Club is currently engaged in establishing a common basis for supporting the future training and professional development of clay specialists through project commissioning. Current topics include the characteristics of water in nanopores, anomalous pore-water pressures, and the behavior of trace elements in clay pore water.

The Crystalline Club (CRC) is a task-oriented expert group. It consists of technical experts (senior experts) with experience in the assessment and/or review of the understanding of crystalline rock as a host rock for deep geological disposal. The CRC fosters the exchange of scientific findings and information related to the safety of repositories in crystalline rock formations. The focus of the work within the Crystalline Club is currently on identifying the chemical conditions of crystalline host rock and the processes that can govern these chemical conditions.

Since national radioactive waste disposal programmes typically span many decades, the OECD/NEA launched the Working Party on Information, Data and Knowledge Management (WP-IDKM) in 2020, involving experts from 26 organisations. The work is carried out by three expert groups addressing the following topics: the Expert Group on Data and Information Management for the Safety Case (EGSSC), the Expert Group on Knowledge Management for Radioactive Waste Disposal and Decommissioning Programmes (EGKM), and the Expert Group on Archiving and Awareness Preserviation (EGAAP). As part of EGAAP the working group on the SER (Set of Essential Records) is to be continued under the leadership of GRS. The key activity of the WP-IDKM in 2025 is the “Symposium on Information, Data and Knowledge Management for Radioactive Waste: Challenges Across All Timescales” Yokohama, co-chaired by GRS.

The JOSA (Joint Sensitivity Analysis Exercise) working group is a voluntary collaboration among several international organizations conducting model calculations in the field of repository research. Its goal is to develop a shared understanding of how to perform and interpret probabilistic sensitivity analyses using various realistic models. To this end, probabilistic datasets from generic or site-specific model calculations are exchanged and independently analyzed by the participating groups using different methods.

The Task Force EBS is an international working group established in 2004 to investigate the performance of bentonite barriers in a deep geological repository in crystalline rock. It is organized into national teams (both European and non-European) under the leadership of the Swedish operator SKB. The core of the work involves modelling to replicate laboratory and in-situ experiments within the framework of specific "tasks." This contributes to enhancing the predictive capabilities of the numerical tools employed and allows for a comparison of results derived from different approaches and methodologies. GRS is currently leading a task on the saturation behavior of confined, compacted bentonite at limited water addition.

CatchNet is an international working group established in 2019 to investigate hydrogeological phenomena in permafrost regions. It is organized into national teams (both European and non-European). Its activities comprise in-situ experiments and model-based analyses conducted within the framework of completed tasks. Within the framework of CatchNet, GRS is currently working on two topic areas. The first concerns experiments on the freezing of water in fractures, with the aim of determining temperature-dependent permeability. The second is related to model-based investigation of the conditions for talik formation during climate cooling and the onset of permafrost.

DECOVALEX-2027 is an international research initiative focused on the modeling of coupled processes. Researchers and experts from 17 different countries and organizations collaborate within this initiative to develop and discuss models and compare them with experimental data. GRS is involved in a specific task with the aim to compare models and methods used in safety assessments for deep geological repositories in rock salt.

2 International developments and co-operation

A key focus of the project's work lies in active participation in international committees and working groups. The objective is to monitor current developments at the international level and to contribute to the further development of strategies, methods, and tools in the field of safety cases for deep geological repositories. In this context, participation in the NEA Integration Group for the Safety Case (IGSC) – including its subgroups, the Salt Club, the Clay Club and the Crystalline Club) – as well as in the NEA Working Party on Information, Data and Knowledge Management (WP-IDKM) is of central importance. In addition, GRS has contributed to the work of other international groups outside NEA as DECOVALEX, CatchNet, EBS Task force and the JOSA exercise. The following sections describe the key activities in which GRS has participated within these bodies.

2.1 Integration Group for the Safety Case (IGSC)

The modern concept of the "safety case" for high- and intermediate-level radioactive waste disposal was introduced in the 1990s by the Nuclear Energy Agency (NEA) through its Expert Group on Integrated Performance Assessment (IPAG). The NEA defines it as "the synthesis of evidence, analyses and arguments demonstrating that a repository will remain radiologically safe without human intervention after closure." The safety case addresses the challenge of assessing and demonstrating long-term safety for geological disposal facilities, taking into account the significant and increasing uncertainties over the period during which the waste remains hazardous /CAP 22/.

Since its introduction, the safety case concept has been further developed by the NEA's Integration Group for the Safety Case (IGSC) – the main technical advisory body to the Radioactive Waste Management Committee (RWMC) – as well as by national programmes in numerous countries. The IGSC has played a key role in advancing and documenting the structure, content and methodologies of safety cases as repository programmes have evolved /CAP 22/.

At present, a growing number of national programmes are advancing towards the licensing and implementation of deep geological repositories (DGRs) for high-level radioactive waste. Licensing represents a key milestone in the iterative development and periodic refinement of the safety case, which typically evolves over several decades through research, site characterisation, design development, safety assessment and integration.

This process is accompanied by regulatory review and continuous stakeholder engagement, and it considers the full lifecycle of the waste, from generation to final disposal. A central element is the systematic optimisation of safety, technical feasibility, sustainability, costs and stakeholder expectations. In this context, the digitalisation of safety cases, as well as effective knowledge preservation and transfer across generations of experts, are increasingly recognised as critical to their successful development and implementation /NEA 26a/.

The safety case concept, as developed by the IGSC and national and international programmes, has reached a high level of maturity. This provides a foundation for further advancements, including the incorporation of operational experience from existing repositories for other types of radioactive waste, insights into operational aspects and waste acceptance, and the transfer of safety case methodologies to alternative disposal concepts. The proceedings of the safety case symposium, see section 2.1.1, give more insight into the evolution of new safety case aspects addressed by IGSC /NEA 26a/.

In 2025 the IGSC celebrated its 25th anniversary. For this event a brochure was created, where IGSC has gathered testimonies and witness statements from many of its expert members on how the IGSC supported their national programmes and their own knowledge of the safety case concept and its complex development. Outstanding experiences like a special conference, symposium, topical session, other event, or any tool from NEA (status reports, databases, figures, flowcharts …) and its importance for the national programme or the own organisation have been highlighted /NEA 25a/.

Key topics of IGSC in 2025 have been the publication of the proceedings of the Safety Case Symposium 2024 in Budapest, the topical session on experiences from operating facilities in safety assessments, safety cases and requirements management, the further establishment of the Next generation network (NGN) in the IGSC and the finalization of the GeneSiS (From Generic to Site-specific Safety Cases) project.

2.1.1 Safety Case Symposium 2024

The NEA Integration Group for the Safety Case (IGSC) Safety Case Symposium, which is held every few years, is a vital platform to discuss the evolution and implementation of safety cases, featuring insights from international programmes at various stages of development. The 2024 symposium was hosted by the Hungarian radioactive waste management organisation PURAM and took place in Budapest from 8 to 11 October 2024.

Ulrich Noseck(GRS) and Manuel Capouet (NIRAS-ONDRAF) the IGSC co-chairs also acted as co-chairs of the Symposium. Under the theme “Moving towards the construction of a safe DGR – Getting real”, the focus was on advancing the construction of safe deep geological repositories (DGRs) for high-level radioactive waste.

While the safety case has become a powerful and essential tool to support decision making for every stage of a geological disposal programme, an increasing number of national programmes have advanced towards licencing and the realisation of their DGR. This progress brings new challenges, e.g. with respect to operational aspects. Optimisation to achieve the best outcomes for safety, technical feasibility, sustainability, costs and to fulfil stakeholder expectations and requirements becomes central. This progress also brings new opportunities, e.g. for learning from experience /NEA 26a/.

The symposium objectives were to:

- Identify the key success factors from safety cases that have supported successful licensing steps, examining the lessons learned and the challenges faced in this regard by advanced DGR programmes;
- Understand how a safety case evolves through the different initial stages of a disposal programme, from the generic to the site-specific stage, and then through the construction stages;
- Explore the role of specific features, such as requirements management systems and information, data and knowledge management (IDKM) in building a safety case and in supporting its evolution throughout successive key milestones in a disposal programme;
- Practically apply knowledge sharing by involving early career scientists in the symposium, enabling them to exchange knowledge and discuss their views, ideas and expectations, with the aim of building an enduring network to support the next generation;
- Exchange experience with other non-DGR nuclear facilities, especially concerning the application of holistic approaches to waste management.

The symposium brought together nearly 200 participants and showcased 94 scientific papers related to above objectives. After welcoming remarks by the Symposium Co-Chairs Manuel Capouet and Ulrich Noseck, the NEA Director-General William D.

Magwood, IV gave an opening speech and Mr. Bálint Nős from PURAM highlighted the role of the safety case in the implementation of the Hungarian national programme in a keynote lecture. The following oral contributions were organised in eight plenary and two times three parallel sessions and accompanied by poster displays and a dedicated poster session. Key input was provided by national programmes advancing towards licensing and realising their DGR's for high-level radioactive waste and by operating nuclear and underground facilities. Topics covered the derivation and management of requirements; the disposal of unconventional and legacy waste; waste from next generation reactors; safety assessment and RD&D; the role of the safety case when moving forward in the face of uncertainty; regulator, implementor and stakeholder dialogue; and updates from national programmes.

In general, the symposium deepened the understanding of how the safety case and its evolution are integrated into repository development programmes, particularly in projects advancing toward construction /NEA 26a/. While the overall structure of the safety case remains stable, it becomes increasingly detailed over time, with growing emphasis on operational aspects. Beyond serving as a "static" demonstration of safety for licensing, the SC is increasingly recognized as a dynamic management tool that continuously tracks safety and links it to repository development, which is further supported by digitalization.

The development of a safety case for disposal is guided by an overarching strategy for radioactive waste management, for which a holistic and graded approach is most effective. Requirements management and systems engineering show strong commonalities across disposal solutions and other industries, underscoring the need for greater knowledge exchange and feedback from experience – particularly regarding operational aspects /NEA 26a/.

Competence maintenance and knowledge transfer is key. Maintaining a network for the next generation and promoting work across generations helps to achieve this. Better understanding the link between management of requirements, change and knowledge may lead to improved multidisciplinary tools such as adequate requirements databases. The interaction with other programmes and initiatives contributes to competence maintenance and knowledge transfer, explores synergies, and provides mutual benefit.

Sustaining competencies and facilitating knowledge transfer are essential. This can be achieved by maintaining professional networks across generations and encouraging intergenerational collaboration. A better understanding of the interplay between requirements, change, and knowledge management could support the development of improved multidisciplinary tools, such as robust requirements databases. Engagement with other programmes and initiatives further strengthens knowledge transfer, fosters synergies, and provides mutual benefits /NEA 26a/.

In summary, the continuation of work on requirements management was mentioned several times on the symposium and it is of particular interest for IGSC members to explore the link between requirements-, change-, and knowledge-management. A second key topic addressed at the symposium is learning from other operating facilities than DGRs, particularly on operational aspects by exploring collaboration with NEA safety division and maintaining collaboration with the expert group EGOS. Both topics have been addressed in the topical session of the 26th plenary meeting in 2025, see section 2.1.2. Current and planned IGSC activities discussed there are illustrated in Fig. 2.1.

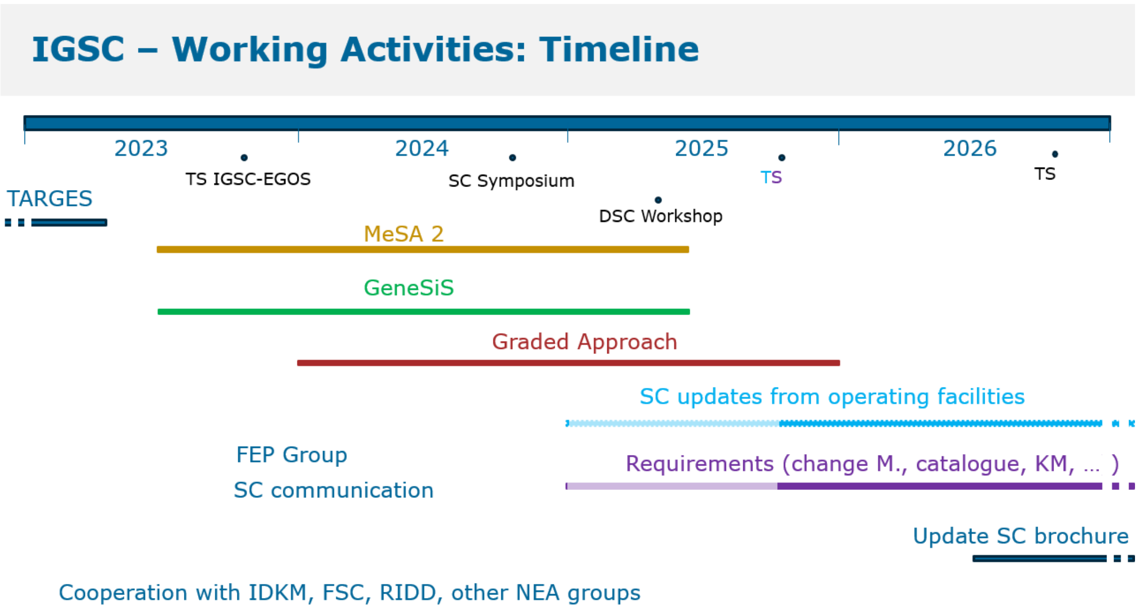

Fig. 2.1 Timeline of key IGSC activities as discussed at the IGSC-26 plenary meeting /NEA 25b/

2.1.2 Topical Session

The topical session of the 27th Plenary Meeting was dedicated to the topic "Safety Assessments, Safety Cases and Requirements Management – Learning from Facilities in Operation or Under Construction". IGSC has recently worked in an ad-hoc group on the "transfer and return of gained experiences on safety cases for disposal facilities

(TARGES)" along five specific topics. Based on this work, presentations and discussions at the IGSC Symposium 2024 and the directly following 26th IGSC plenary meeting, two aspects have been selected for the topical session of the 27th IGSC plenary meeting: (1) Learning from Updating the Safety Assessment (SA) & Safety Case (SC) of Facilities in Operation and (2) The Role and Evolution of Requirements and Configuration Management (RCM). The session explored experiences, good practice, and issues in existing disposal facilities. Target disposal facilities for knowledge exchange included near-surface disposal facilities, geological facilities in shallow depth, and constructed or existing DGRs /NEA 26c/.

The objectives were (1) to learn about the experiences for updating SA and SC of facilities in operation; identify good practices that can be transferred to DGR community; (2) to understand how RCM is used and evolves from early stages of a project to a facility that is built or operated; and (3) to identify commonalities and differences between operating facilities and planned DGR's with respect to SA and SC updates and RCM setup and evolution, and deduce findings useful for DGR projects.

The speakers were encouraged to share their experience related to the role and evolution of SA/SC/RCM along the development and life cycle of their facilities. Of particular interest are experiences related to specific milestones, rapid or unexpected changes – be it due to external or internal events – and about lessons learned. A bundle of questions have been send to the speakers in advance /NEA 26c/:

Overall, the questions aimed to understand how safety analyses (SA) and safety cases (SC) have evolved and kept up to date following the licensing of a facility. One focus was on the reasons driving such updates, for instance, regulatory changes, technical adjustments, operational experience, or new insights regarding the facility or its inventory, and which parts of the safety case are affected by them.

Furthermore, utilization of data and experience derived from construction, operation, and monitoring activities to refine models, validate assumptions, and reduce uncertainties have been gathered. In this context, consideration was also given to the difficulties that may arise during the introduction of new methods, models, or computational tools, for example, regarding consistency with previous analyses or the availability of additional data, and how these challenges were resolved. The questions also addressed how potential discrepancies between the original safety case submitted for licensing and subsequent updates are managed. Closely linked to this is the question of how knowledge, including data, models, tools, and expertise, is organized, preserved, and transferred over the long term, and what role research and development plays in the continuous improvement of safety analyses.

As mentioned above the second central aspect of the topical session was also Requirements and Configuration Management (RCM): The questions should examine how this system evolves across the various phases of the repository project, how it handles design changes or unexpected events, and how it contributes to ensuring consistency among requirements, facility design, and the safety case. Likewise, the extent to which RCM supports other processes, such as risk-informed decision-making or intergenerational knowledge management, is examined, along with the tools employed for this purpose, including potential linkages with digital safety cases or international databases.

The topical session comprised 10 presentations from 8 countries and was closed with a final discussion. Some key conclusions with regards to updating the Safety Case and Safety Assessment of facilities in operation, are the following. For more details, see /NEA 26c/:

- Changes and updates are normal since facilities are optimised or adapted. Common triggers for updates of SA/SC could be /NEA 26c/:
    - Regulatory requirements – periodic safety reviews, changes in regulation
    - Design optimisations or adaptations
    - Changes in waste sorts or streams
    - R&D achievements, new knowledge
    - New data, including monitoring data, that e.g. indicates unexpected phenomena
- Approval by the regulatory authorities of changes in the SA/SC is usually not a problem as long as SA/SC or changes are thoroughly justified and well documented
- Updates do not always lead to reduced conservativity – needs expectation management and adequate stakeholder communication
- R&D after licensing is necessary to reduce uncertainties and optimize the facility and need to be reflected in SA/SC updates. Here, communication between implementer and regulator is needed.

- In-house knowledge management is important, particularly for traceability of decisions and underlying assumptions. This issue is addressed in requirements management.

The outcome of the topical session serves as input for the planning of further activities, including joint efforts between IGSC and other NEA groups. A summary report is published on the IGSC webpage /NEA 26c/.

2.1.3 Next Generation Network (NGN) of the IGSC

In 2024, the IGSC has identified the need to involve early career scientists in its key processes and working groups, to ensure a transfer of knowledge and the consideration of the younger generations´ views. This lead to the formation of the Next Generation Network (NGN) which consists of emerging experts from implementing organisations, research institutions, and regulatory agencies.

Members of the Programme Committee of the IGSC Safety Case Symposium 2024 hosted the first virtual meetings of the network and gave a webinar about the safety case. Later meetings were organized by the NGN members themselves. The NGN was involved in the organisation of the Young Professional Session of the IGSC Safety Case Symposium 2024 in Budapest and provided two of its chairs. The presentations in this session intended to give advice to young professionals about the safety case, particularly targeting knowledge transfer from one generation to the next. Questions gathered by the NGN were the basis of the panel discussion and the wrap-up session at the end of the symposium included feedback from the young professionals' perspectives. Other activities included the first in-person meeting before the start of the symposium, posters (e. g. /BRU 26a/, /ELF 26/, /GEH 26/, /MOL 26/, /PAY 26/, /RIM 26/) and an oral presentation /BRU 26b/ by members of the NGN.

The overall impression during the IGSC Safety Case Symposium 2024 was that the safety case community is open and welcoming to a network of young experts and sees its value and necessity for knowledge transfer and continuing international collaboration. Therefore, the NGN continued its work after the symposium with the aim of expanding its network and establishing itself as part of the safety case community. To this end, it sought recognition as an official ad hoc group under the auspices of the IGSC, which was achieved at the IGSC-27 Plenary Meeting in Paris in October 2025 for a duration of four years. This includes the allocation of one seat in the IGSC core group for an NGN member.

The NGN serves as a professional platform designed to address a pressing challenge: the long-term sustainability of expertise in the development of safety cases for radioactive waste disposal. By offering a forum for collaboration and learning, the NGN supports early-career professionals while fostering connections across disciplines and organizations. To fulfil its missions, the NGN ad-hoc group aims to:

1. **Support professional development:** Create opportunities for early-career professionals to deepen their expertise in safety case development, gain insight into the international methodologies and learn from good practices in the field.
2. **Integrate emerging voices into the community:** Act as bridge to introduce perspectives and contributions from the next generation into the broader safety case dialogue, ensuring their active involvement in ongoing discussions and activities.
3. **Promote structured knowledge transfer:** Facilitate mentorship, peer-learning, and other means to ensure long-term retention, transfer, and practical application of expertise withing the safety case community.
4. **Build diverse professional networks:** Connect professionals across technical and non-technical disciplines, such as sciences, engineering, social sciences, risk assessment, and policy, to foster interdisciplinary collaboration and knowledge exchange.
5. **Enhance visibility and awareness:** Showcase the contribution of early-career professionals through NGN activities at relevant conferences, organize dedicated sessions for emerging experts, and advocate for early engagement in knowledge transfer.

The GRS is strongly involved in the work of the NGN as Anne Gehrke belongs to the network since its foundation and is member of the NGN core group. The core group organizes virtual and in-person meetings, provides a newsletter, circulates important information, and maintains contact with NEA and IGSC.

The activities of the NGN included taking on the role of rapporteur during the Expert Group on Operational Safety (EGOS) Webinar 2025 “Co-activity in Underground Repositories” and during the topical session at the IGSC-27 Plenary Meeting 2025. Furthermore, the NEA/IGSC/NGN concept was presented at the safeND /GEH 25/ and at the EURAD-2´s Lunch & Learn Session on 17 December 2025 /TIL 25/.

For 2026, an in-person meeting of the NGN and participation at the IGSC-28 Plenary Meeting is planned as well as the organization of a series of expert sessions. Furthermore, requests have already been made by IGSC for participation of NGN members in various working and ad-hoc groups.

2.1.4 GeneSiS project

The Integration Group for the Safety Case (IGSC) launched in 2024 the Generic to Site-Specific Safety Cases (GeneSiS) project to support the development of generic safety cases and the transition to site-specific safety cases, particularly for member countries at less advanced stages of their DGR programme. It intended to

- provide a community of practice in which participating organisations can learn from the experience of more advanced programmes who have already completed elements of this transition;
- produce guidance about which areas to focus on at different stages of the programme, what approaches are and are not suitable at different stages and how the approach may evolve as the programme progresses; and
- produce generic products that can be adopted and used as a common and internationally tested starting point for safety case and design development.

The results of the project will be published in three major reports, /NEA 26d/, NEA 26f/ and /NEA 26g/.

One objective of the GeneSiS project was to develop guidance regarding the various approaches available for key topics in the safety case, as well as essential considerations and best practices for selecting an approach. In particular, it has been analysed, how these aspects evolve from the early pre-concept stage to the final design stage, where comprehensive site-specific information is available. To support comparison and analysis across different countries, the GeneSiS project defined three safety case stages, covering the timeframe of transition from generic to site-specific: pre-concept, initial concept and de-tailed concept. A questionnaire addressing key safety case topics was created and used as a framework for structured interviews with countries at different stages of the DGR pro-gramme, allowing learning from their positive and negative experiences /NEA 26d/.

After the evaluation of interviews with the organisations from countries advanced in their DGR programmes, namely with Andra, Nagra, Posiva and SKB, in 2025 additional interviews were conducted with organisations from countries with less advanced programmes, i.e. BGE, NUMO and NWMO. Responses were analysed to identify similarities and differences in approaches between countries and programme stages and explore trends in how the different aspects of the safety case evolve as the programme progresses. The information from all interviews is evaluated and summarized in a report "Generic to Site-Specific Safety Cases (GeneSiS) – Safety Case experiences from implementer organisations and topic-specific guidance" /NEA 26d/, which presents the key lessons learnt from the interviewed organisations, across each of the safety case topics discussed, and uses them to formulate recommendations for the safety case at different stages in the repository programme. Beside some general aspects the following safety case topics have been evaluated and are discussed in detail in the report. Some general statements are given here:

- The **Safety Concept** describes why the repository is safe, which will be achieved through the interplay of natural and technical barriers and their safety functions (primarily containment and isolation). The specific design depends heavily on the host rock and the waste.
- **Requirements Management** strongly contributes to knowledge management. The early definition and systematic management of requirements ensure the traceability of decisions. Requirements are country-specific; while international experience can be utilized, they must be adapted to local conditions.
- **Safety and Performance Indicators** serve to demonstrate that all barriers function as intended and that the repository as a whole is safe (e.g., risk/dose limits, barrier performance).
- **Features, Events and Processes (FEPs)** are the foundation for safety analyses and scenarios, ensuring the comprehensiveness of the assessment. Databases are useful early on and become site- and concept-specific requirements later in the process. Development, care and updating are resource-intensive.
- **Scenarios**: are a central tool for evaluating uncertainties over long timeframes, typically categorized in reference and alternative scenarios, and "what-if" cases. As the repository project evolves, comprehensive scenario coverage becomes increasingly important.
- As the repository programme progresses from generic to site-specific, **modelling** approaches also evolve, e.g. becoming more representative, and probabilistic

studies usually gain more importance, since more reasonable data are becoming available. Quality assurance through comparisons and benchmarking is crucial.

- For **Data and Model Management** standardized procedures (e.g., data release/freezing) established early in the programme, ensure consistency, transparency, and traceability.
- **Waste Acceptance Criteria (WAC)** should be planned and documented early on, initially adopting a conservative approach. Engaging waste generators is essential to avoid the need for subsequent adjustments.
- **Communication** evolves across the project phases: In general, this develops from explaining basic principles in the early stage to providing transparent information during site selection and to engaging in detailed dialogue with informed stakeholders at later stages. A consistent structure for safety assessments is recommended.

All detailed analyses and discussions will be published in the final report end of 2026 /NEA 26d/.

2.2 Salt Club

The “Expert Group on Repositories in Rock Salt Formations (Salt Club)” was established in 2012 by OECD/NEA. Current member states are the United States, Germany, the Netherlands, United Kingdom, Poland, Australia and Romania. The key objective of the Salt Club is to promote the exchange of information and share approaches and methods to develop and document an understanding of salt formations as a host rock for a high-level radioactive waste repository. The Salt Club holds regular annual meetings at which its Programme of Work (PoW) is established, updated and reported about. In the current PoW of the Salt Club the following work activities are listed:

- Common Features, Events and Processes (FEP) catalogue for a HLW repository in rock salt and Salt Knowledge Archive (scope, definition, collection of ideas, and available information on state-of-the-art of knowledge management);
- Scenario development and consequence analysis as part of the overall safety case for repositories in salt;
- State-of-the-art report on important commonalities and differences between repositories in flat bedded and domal salt;

- Geomechanical integrity evaluation, including numerical, experimental, and field-work on the evolution of both the excavation damaged zone and granular salt backfill;
- Thermodynamic aspects of brine chemistry
  - Actinide and Brine Chemistry (ABC) Salt Workshops;
  - Thermodynamic Database (Pitzer)
  - Research on actinide-organic interactions.
- Microbial gas generation in saline systems; and
- Lessons learned from failure events and processes in conventional salt mines.

Main activity of GRS was the participation in the NEA Salt Club Working Group "The role of scenarios in the modelling strategy for the safety assessment for deep geological repositories". To assess the influence of a deep geological repository (DGR) on humans and the environment, in many countries, timeframes of one million years must be taken into account. Due to these long timescales and the complex environment of a DGR the assessment of its influence requires numerical modelling using the following modelling strategy consisting of four stages /NEA 91/, /NEA 12/:

i. derivation of a conceptual model,
ii. quantitative formulation of the accompanying mathematical model,
iii. transfer of the mathematical model into a numerical model and
iv. qualification of the model.

This is a quite common scientific approach and there is wide consensus on this modelling strategy to perform a safety assessment for a DGR /NEA 12/. When modelling a complex system such as a deep geological repository, simplifications in the modelling processes are unavoidable, especially at the stage of developing numerical models (stage iii). The challenges to deal with data and model uncertainties are well known to the scientific community and there is a wide range of recommendations how to manage these kinds of uncertainties, e.g. /EPA 09/, /NEA 12/.

Scenarios are abstractions of collections of FEPs that do not include explicit causality and timing of when actions occur. Scenarios simplify what occurs in a repository, rather than considering an explicit fault and event tree associated with each possible future occurrence in a repository. As part of the conversion from scenarios to assessment implementations, the timing and causality of everything in the conceptual must be added in.

One of the specific challenges for the safety assessment for a DGR are the considered long timescales. Due to these timescales the uncertainties regarding the evolution of the repository system are significantly higher than in most other scientific fields using the modelling strategy above. In addition to data and model uncertainties, scenario uncertainties must be considered, especially those related to climatic evolutions. Scenario uncertainties usually dominate data and model uncertainties and, therefore, instead of one predicted evolution a set of scenarios is to be addressed in the safety assessment to deal with these scenario uncertainties. The scenarios are based on a wide range of features, events and processes (FEP), that are potentially relevant for the evolution of the repository system. The scenario approach is used in other fields, too, but the considered timescales are mostly in the order of several decades. The scenario approach is applied in all national programs installing a DGR and since the scenarios build the fundamental basis for the quantitative assessment, comprehensive recommendations exist, how to deal with scenario uncertainties in the safety assessment for a DGR /VIG 07/, /NEA 12/, /IAEA 12/, e.g.:

Regardless of the method used for developing the scenarios, all features, events and processes that could significantly influence the performance of the disposal system should be addressed in the assessment. (…) Hence, it should be shown that all potentially significant migration pathways from the facility have been considered and that possible evolutions of the system have been taken into account /IAEA 12/.

The set of scenarios covers the uncertainties of the future evolution of the repository system, but it is not clear how the scenario approach is linked to the modelling strategy. Recommendations how to deal with scenario uncertainties in the modelling strategy for timescales up to one million years are non-existent. On the other hand, regulations require exactly the presentation and justification of the linkage between scenarios and the numerical models, e.g. the German regulation for the calculation of the effective dose /BASE 22/:

It must be clearly shown how the scenarios are mapped in the models used and parameterized. The properties and parameters used must be presented and justified, taking into account the alternatives. For the implementation in calculation cases for dose estimation, it must be ensured that the evolutions determined over the assessment period of one million years are consistent and comprehensive with regard to the potential release of radionuclides from the repository.

Each safety case contains an argumentation that the models applied meet the requirements of the scenarios. Whether this argumentation meets the requirements of the regulator and other stakeholders cannot be assessed across the board. However, it makes sense to attach more effort to this aspect to build a comprehensible and traceable safety case. Therefore, the Salt Club starts an activity with the objective to investigate possibilities for mapping scenarios to the numerical models (or vice versa) by investigating national programs for repositories in salt.

To start the activity a questionnaire has been developed investigating experiences and possibilities of the linkage between scenarios and the modelling procedure. The following questions are to be answered:

Introductory section (regulation context):

- How long is the assessment period? Is a probabilistic approach required? If yes how are probability density functions (pdfs) quantified?
- Which kind of models do you use for your safety assessment? How are they developed?
- What data do you need?

Main section:

- How are the FEP and/or scenarios used in the modelling process?
- Is a systematic approach applied?
- Is there any documentation of this usage/approach?
- Is it possible to map scenarios consistently to the different stages i) to iii) in the modelling process?
- Is it possible to use scenarios to qualify the applied models (stage iv)?)
- Is there a check, whether all FEP/scenarios are used in the modelling process? If yes, what follows, if the check is negative? Is there a feedback loop to the management of scenarios, especially the categorization of scenarios?

2.3 Clay Club

Between 2024 and 2026, the NEA Clay Club made significant progress in the scientific understanding of clay-rich (argillaceous) rock formations as host rocks for the geological disposal of radioactive waste. In 2024, the focus was on strengthening international cooperation and initiating new research projects. A key event was the Porewater Workshop in Bure (France), which substantially deepened the understanding of pore-water chemistry and its significance for repository safety. Additionally, an international project on pressure anomalies was launched, laying the groundwork for a systematic analysis of pore-pressure conditions in clay formations. In 2025, the results of the CLAYWAT project have been published. They yielded new insights into water behavior within nanoscale pore spaces and highlighted the importance of restricted transport processes /NEA 25c/. Furthermore, the Clay Club focused intensively on trace elements in clay formations and their role in geochemical processes and safety analyses.

The project on pressure anomalies yielded key insights during the 2025–2026 period. An investigation of 14 international sites revealed that underpressure prevails in clay formations, primarily resulting from geological unloading processes such as erosion and glacial retreat. The persistence of these anomalies depends significantly on formation parameters, such as thickness and hydraulic diffusivity. Methodological advances, specifically the development of diffusion and radial flow models, improved the interpretation of measurement data and the estimation of undisturbed pressure conditions. These approaches underscore the importance of long-term monitoring for reliable subsurface characterization. Overall, the results confirm the fundamental suitability of clay formations as natural barriers for the deep geological disposal of radioactive waste. At the same time, it is evident that site-specific differences and complex coupled processes necessitate detailed analysis. Future work will focus particularly on the influence of sedimentation and diagenesis on long-term evolution.

2.4 Crystalline Club

The “Expert Group on Geological Repositories in Crystalline Rock Formations (Crystalline Club, CRC)” was established in 2017 by OECD/NEA. Current member states are Australia, Canada, Czechia, Germany, Japan, Romania, Korea, Spain, Switzerland and USA. The CRC promotes the exchange of information and shares state-of-the-art approaches and methods to improve the understanding of crystalline rocks as a host rock for a high-level radioactive waste repository. The CRC is a task-oriented expert group. It is composed of senior technical experts with experience in evaluating and/or reviewing the understanding of crystalline rock as host rocks for deep geologic disposal projects. Members represent waste management agencies, regulatory authorities, academic institutions, and research and development institutions. The CRC is managed by its Bureau, including a Chair, a Co-Chair and several Vice Chairs.

During 2024 and 2025, the CRC addressed two main topics:

1. Identification of chemical conditions important to crystalline repository performance and their impact on canister corrosion
2. Scoping the feasibility of developing a catalogue of characteristics of crystalline rocks

The main goal of the CRC Program of Work (PoW) 2023 – 2024 was to identify crystalline host rock chemical conditions relevant to crystalline repository performance and to identify processes that may control those chemical conditions. It was intended to include their impact on canister corrosion whenever results are available.

The properties and location of a crystalline host rock have direct effects on chemical conditions at the depths of a potential repository. In turn, chemical conditions at repository depth have direct effects on waste package degradation rates, waste form degradation rates, buffer performance, and radionuclide solubility and transport. Therefore, a good understanding of chemical conditions in crystalline host rock and how they could evolve over time is needed for effective crystalline repository performance assessment.

The selection of suitable canister materials for repositories in crystalline rock is dependent on the geochemical conditions in the host rock formation. The corrosion behaviour under the conditions of the near field is one of the main parameters influencing the selection of suitable canister materials, and canister design / canister concepts have to be developed in order to avoid corrosion processes.

The project was divided into two tasks:

- Task #1: Identification of chemical conditions important to crystalline repository performance and their impact on canister corrosion
- Task #2: Curation of a list of publications that improve understanding of those chemical conditions, how they are controlled, how they originate, and how they may evolve due to repository perturbations and global temperature cycles. The list of publications will include available literature on models that have been developed to simulate and

predict chemical conditions as well as literature on canister materials and canister corrosion.

To address the task, an international geochemistry literature working group was set up and worked on the task during the years 2023 and 2024. Organization and communication was realized via e-mails and virtual working meetings. For the compilation of a list of publications, the online Mendeley reference manager was used. An international working group has compiled and reviewed a reference database with more than 600 entries during the years 2023 - 2025. The project was finalized in 2025. It is planned to transfer the CRC Geochemsitry Literature Database project (Cryschem) from the Menedeley platform to GitHub and to publish the reference database together with an associated summary report in 2026. The report describes and provides a summary of the database, highlighting research from CRC and non-CRC countries.

On 1-3 July 2025, the CRC-8 Plenary Meeting was held in-person in Rauma, Finland (co-hosted by POSIVA). The focus of the meeting was on updates on the Country Programme and R&D status of the member countries, the finalization of the Programme of work for 2025-2026 and on the topical session. The topical sessions of Crystalline Club meetings are associated with the main goal of the CRC Program of Work. In CRC-8, each national delegation was invited to present on a topic of interest within its national program. It was aimed at giving the opportunity to highlight specific technical topics and open questions. The presentations in the topical session were supposed to help to identify topics of common interest for the future Programs of Work of the CRC, end specifically for the PoW 2025 – 2026.

Following the presentations a brainstorming session allowed the members to discuss the content of the proposed new topics for the PoW 2025 - 2026. The Crystalline Club then decided to send a call for champions to lead the topics and further complete an online survey to rank the proposals.

Crystalline Club decided in a Bureau Meeting on 09 October 2025 to proceed with the topic of “Scoping the feasibility of developing a catalogue of characteristics of crystalline rocks”, chaired by NWMO/Canada. The associated working method is:

- Task #1: Undertake a “lessons learned” exercise with key individuals involved with the Clay Club catalogue compilation to understand pitfalls, challenges, and opportunities with such an endeavour.

- Task #2: Summarize the outcome of Task #1 in a CRC internal technical document, determining the feasibility of moving forward with the project to develop the database. If moving forward is deemed feasible, this document would also include a proposed roadmap for subsequent PoW.

The main output for the initial programme of work will be a concise technical document describing the outcome of task #2 above. The summary document would provide direction for embarking on a subsequent program of work, if it is determined to be a feasible endeavour. It is envisaged that the initial POW would continue until the end of 2026, or early 2027, and the second POW would be initiated early in 2027. One of the future challenges is to thoroughly examine whether developing a catalogue of characteristics of crystalline rocks is feasible. If it turns out to be too challenging for CRC to realize, a new PoW has to be identified for 2027 – 2028.

The 9th Plenary Meeting of the CRC is planned in-person in June 2026, in Toronto, Canada, co-hosted by NWMO. The focus of the topical session will be on the feasibility to develop a catalogue of characteristics of crystalline rocks (PoW 2025 – 2026).

The Crystalline Club remains committed to enhancing its visibility and broadening the scope of technical initiatives within its ongoing programs of work. The CRC is looking forward to further maturation as an expert group through 2026 and beyond.

2.5 Working Party on Information, Data and Knowledge Management (WP-IDKM)

Radioactive waste emerges from a diverse range of sources, spanning the entire nuclear fuel cycle and various applications in industry, medicine, defence, and research. Regardless of whether a nuclear fuel cycle is closed or open, the waste requires interim storage before its ultimate placement in a deep geological repository. Throughout this complex lifecycle, an extensive volume of data and information is generated. Recognizing the challenges of managing this critical information, many countries are now investigating the development of a digital safety case – an innovative approach to comprehensively tracking and documenting radioactive waste management processes. Nuclear power generation facilities operate over multiple decades, while nuclear waste disposal sites have even more extended timelines. This longevity presents complex challenges that stretch across several generations of workers and technological developments.

Maintaining comprehensive and structured records becomes crucial—not just of the waste itself, but also of its packaging, processing, and management strategies. These detailed records serve a critical purpose: they ensure that future decision-makers can effectively manage the hazards associated with nuclear waste throughout its entire lifecycle. Moreover, the nuclear waste management community now recognizes the importance of developing strategies that preserve awareness of waste repositories and disposal facilities over extremely long periods.

Technological advances have simultaneously simplified and complicated this challenge. On one hand, modern technologies enable the generation and querying of vast amounts of data with unprecedented ease, provided the information is appropriately structured. On the other hand, these same technologies introduce new complexities, such as the risk of digital obsolescence, which can threaten long-term information preservation. The key lies in creating robust, adaptable documentation systems that can withstand technological shifts and generational changes, ensuring critical knowledge about nuclear waste management remains accessible and comprehensible for decades and potentially centuries to come.

In 2020, the OECD Nuclear Energy Agency (NEA) established WP-IDKM) to coordinate these activities in a more holistic way, considering cross discipline and cognoscente of all timescales of the information cycle. WP-IDKM was established in the footsteps of the former NEA initiative on the Preservation of Records, Knowledge and Memory (RK&M) from 2011-2018. WP-IDKM was comprised of four Expert Groups covering the structuring of data, information and knowledge when developing a safety case, knowledge management across generations, archiving, and long-term awareness preservation. Among them were the Expert Group on Archiving for Radioactive Waste Management Activities (EGAR), and the Expert Group on Awareness Preservation after Repository Closure (EGAP) to focus on archiving and awareness preservation specific tasks. After two successful mandate periods, the WP-IDKM decided to merge both groups in 2024 to enhance future cooperation in both areas of work and identified topics of common interest. The new expert group on archiving and awareness preservation (EGAAP) was created. Three broad areas are addressed in EGAAP, namely the Key Information File (KIF), the Set of Essential Records (SER) and supporting work activities including future literacy.

2.5.1 NEA Symposium on Information, Data and Knowledge Management for Radioactive Waste: Challenges Across All Timescales

The Nuclear Energy Agency (NEA) Symposium on Information, Data and Knowledge Management (IDKM) was held in Yokohama, Japan, in October 2025. It brought together technical and non-technical experts, policy and decision makers, waste management organizations, regulators and interested parties. The symposium was based on the current work of the NEA Working Party on Information, Data and Knowledge Management (WP-IDKM).

Many countries are implementing strategies for the permanent disposal of radioactive waste through geological disposal and are currently assembling the scientific underpinning to demonstrate that such facilities will be safe during both operations and after closure. Radioactive waste management (RWM) is particularly demanding in the area of IDKM due to:

- the volume and multidisciplinary nature of the specialist information, data and knowledge produced;
- the requirement to operate within robust regulatory frameworks;
- the extended duration of national programmes, with geological disposal facilities often planned to operate for in excess of one hundred years; and
- the need to preserve records for very long periods of time to ensure the confidence of future societies.

In recent years, there have been significant developments in IDKM, both relating specifically to the field of radioactive waste and in other fields. On that basis it was decided to hold a Symposium on IDKM for Radioactive Waste and Geological Disposal, which provided a forum to discuss these advancements, and further develop the holistic vision on IDKM practise for radioactive waste. In other words, the management and safe disposal of radioactive materials is not merely a technical task – it is a cross-generational responsibility. The information we collect, structure, and preserve today must remain understandable, accessible, and trustworthy for decades and even centuries to come to ensure informed decisions can be made to manage the waste hazard effectively until its disposal. Moreover, even after disposal, there is now a consensus on the importance of adopting strategies to preserve awareness of waste and disposal facility for long periods of time. This requires not only robust technical systems, but also a deep understanding of societal processes, digital sustainability, and international collaboration.

The symposium provided the possibility to present and discuss significant developments in IDKM in RWM in a wider international frame in this symposium. It allowed NEA member countries to present their internal initiatives and learn from the experience of others; enhanced the understanding of IDKM among stakeholder groups and RWMO's, fostering dialogue and feedback; united IDKM and information technology specialists from the nuclear and non-nuclear sectors to understand the state-of-the-art technology and enable horizon scanning and enabled networking and knowledge exchange. It contributed to build an international consensus on IDKM best practices for radioactive waste management, to develop a holistic vision of IDKM across technical and non-technical stakeholders across all timescales and identified future challenges on IDKM that would benefit from future international co-operation.

Key Topics of the Symposium were

- Technological Innovations: AI, semantic technologies, and digital safety cases
- Stakeholder and Societal Involvement: Expectations, communication, and intergenerational knowledge
- Awareness preservation: approaches and strategies
- Data structures and archiving techniques for the long term
- International Collaboration: Exchange of best practices
- Holistic view to IDKM for RWM/decommissioning

The publication for the proceedings is envisaged for autumn 2026 (NEA, 2026a).

2.5.2 The Set of Essential Records (SER)

The SER can be understood as a collection of the most important records about a facility and its waste, selected from the vast number of records produced during the lifetime of the repository, and intended for permanent preservation /NEA 19/. Since records are produced during all phases of a repository programme, the development of the SER will be an ongoing process that should be under continuous maintenance and be regularly reviewed until repository closure. The SER aims to provide sufficient information for current and future generations to ensure an adequate understanding of the repository system and its expected performance. This will enable responsible parties to review and verify the repository performance and make informed decisions regarding the repository. The SER should serve as a source of detailed data and information on the repository system, primarily for specialists and researchers, as well as for decision makers, regulators and other authorities (noting its volume, technical language and accessibility). To allow future generations to efficiently discover the information, search tools based on international archival description standards as well as an explanation document should be part of the SER. It is crucial that the most recent and approved version of the SER is made available in the dedicated archive/information centre /NEA 19/.

Within the expert group EGAAP the approach of the set of essential records is currently further developed. There are particularly two major tasks, namely (I) to investigate the SER as tool for knowledge capture and (II) to evaluate how application of advanced technologies, namely AI tools can contribute to foster SER selection and management.

With respect to the former task the NEA Expert Groups on Archiving and Awareness Preservation (EGAAP) and on Knowledge Management for Radioactive Waste Management Programmes and Decommissioning (EGKM) have just started a collaboration to investigate how knowledge management activities and the concept of the SER can profit from each other. In particular, the questions to be addressed are: how non-codified, essential, knowledge held by staff can be managed and included into the SER; and how can the SER also help staff in identifying and accessing essential available knowledge? /NOS 26b/

The mapping and essential analysis of knowledge can serve as a complementary basis for prioritising and organizing the processing of records, leading to the identification and capitalisation of key non-codified knowledge (identifying, structuring then codifying key knowledge that is not yet documented in records). The SER targets a technical expert audience, providing future generations (over shorter and longer timescales) with detailed knowledge about the repository, the materials consigned to it, their origin, how they got there and why it is safe. In this respect, the SER supports identifying essential knowledge, codifying it and transferring it to those who need it. During construction and operation of the repository, the SER will be a ‘live record set’, which will be added to and maintained as new knowledge is generated, cf. Fig. 2.2. During this time, the SER could serve as a knowledge base, allowing employees within any organisation engaged in radioactive waste management to quickly identify, find and access key records related to specific topics like e.g. the characteristics of the geology, the waste, the engineered barrier system, and the safety assessment /NOS 26b/.

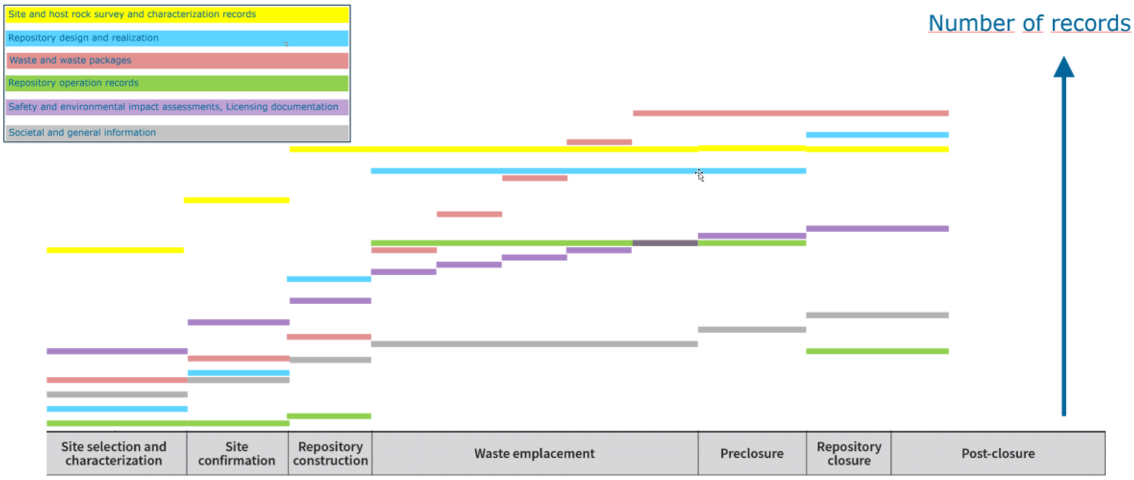

Fig. 2.2 Evolution of the SER during repository lifetime /NEA 26g/

The second task is further described in section 2.5.3.

2.5.3 AI applications supporting the SER approach

The identification of SER-relevant information is a primarily manual, expertise-driven process, that is highly resource-intensive. It relies heavily on individual experience, tacit knowledge, and contextual understanding, while the underlying document collections often lack standardized metadata, consistent versioning, or explicit links between documents, decisions, assumptions, and safety arguments. This situation poses a growing risk that relevant information may become difficult to find, interpret, or contextualize over time, particularly for future generations that will not have access to today's experts.

At the same time, recent advances in artificial intelligence, particularly methods based on natural language processing, machine learning, and semantic analysis, have demonstrated significant potential for supporting large-scale document analysis. In fact, modern AI-based systems can perform semantic searches that go beyond keyword matching, extract structured information from unstructured text, and operate consistently across thousands of documents.

In this regard, considerations have been taken to explore how artificial intelligence can be used in a responsible and regulatorily compatible manner to support Information, Data and Knowledge Management (IDKM) tasks related to the identification, handling, and long-term preservation of safety-relevant information in the context of radioactive waste repositories, with a particular focus on the Set of Essential Records (SER). The underlying motivation is not to automate expert or regulatory decisions, but to improve transparency, consistency, and traceability in dealing with very large, heterogeneous, and often poorly structured document collections that have accumulated over several decades.

However, experience also clearly shows that purely generative approaches based on large language models (LLMs) face fundamental limitations in safety-critical and highly regulated environments. These include the risk of hallucinations, insufficient inherent traceability of results, limited explainability, sensitivity to input quality (such as OCR errors), and a lack of regulatory acceptance.

Against this background, the initial aim was to examine how AI can be used as a controlled and transparent tool to support decision-making in SER-related activities. The goal is not the automation of SER selection, but the provision of structured, traceable, and reproducible support for experts who remain responsible for final classification, validation, and approval.

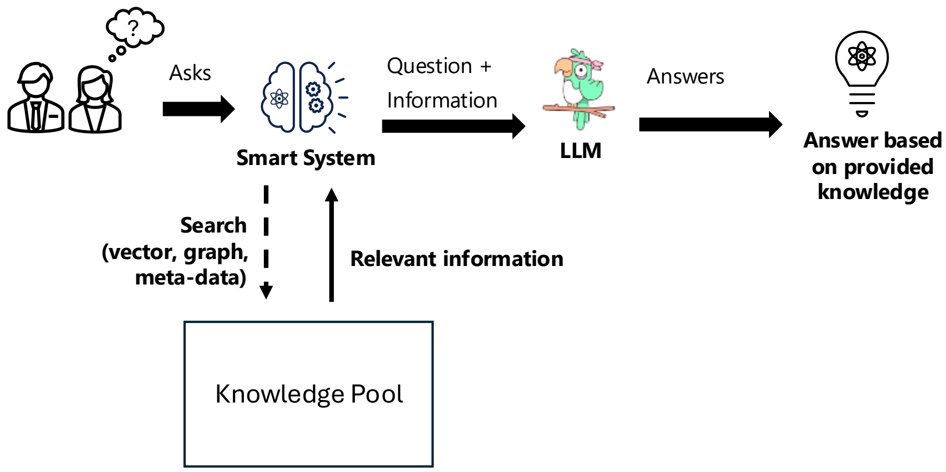

Fig. 2.3 Principle structure of retrieval of information from knowledge pool /DIE 26/

As a methodological starting point, GRS has developed a structured approach for the use of artificial intelligence in IDKM, especially within safety-critical and highly regulated environments (/DIE 26/). This approach is not limited to generic IDKM applications but is explicitly suitable for the use in the context of the Set of Essential Records.

A central element of this approach is the assumption that AI must operate within a knowledge-driven and provenance-controlled architecture (Fig. 2.3). Instead of applying generative models directly to raw document collections, GRS follows a concept based on a semantic knowledge pool. This knowledge pool integrates several layers (Fig. 2.4): Original documents and extracted text fragments form the Content layer. Controlled metadata capture provenance, lifecycle phase, version status, and SER-relevant attributes in the Metadata Layer. A semantic layer based on ontologies and knowledge graphs explicitly models relationships between technical concepts, regulatory requirements, decisions, assumptions, and safety arguments. Finally, the Access Layer provides semantic retrieval and AI-assisted interfaces. Within this architecture, AI functions are deliberately constrained by validated and contextualized knowledge, which significantly enhances transparency and auditability.

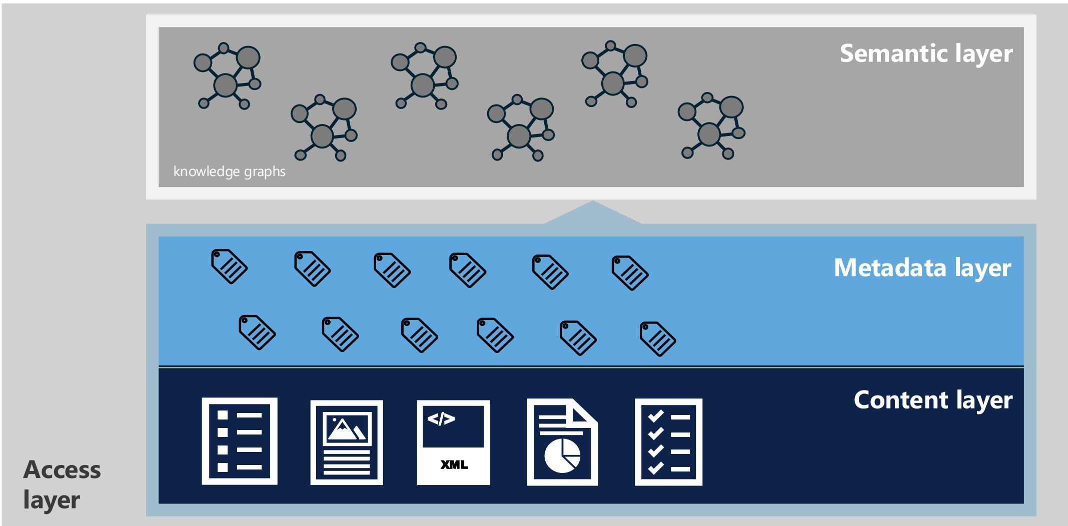

Fig. 2.4 Semantic Knowledge Pool (/DIE 26/)

Based on this methodological foundation, a set of SER-related use cases were identified to be investigated. GRS started to address the question of how advanced tools can support the identification and selection of records for the SER from the large number of reports created for the ILW/LLW repository Konrad.

The anticipated investigations are intended to be carried out within a dedicated project group comprising contributions from GRS, BGE, PURAM, and academic partners, in particular the Harz University of Applied Sciences. GRS contributes the methodological framework for AI-supported IDKM and coordinates the conceptual work, while BGE provides repository-specific expertise and access to the Konrad document base. Academic partners and international contributors support the exploration and evaluation of AI-based methods from a scientific perspective. This interdisciplinary composition is intended to ensure that the planned investigations address both, practical repository requirements and methodological robustness, while remaining firmly embedded in an expert-driven and regulatorily aligned context.

First use case focuses on the re-analysis of records that have already been manually classified as SER or non-SER. By comparing AI-supported analyses with existing expert decisions, it is intended to examine the extent to which semantic indicators, extracted content elements, and document characteristics identified by AI correspond with established SER assessments. This comparison serves both as a validation of the approach and to identify systematic patterns and potential inconsistencies.

A second use case addresses the thematic and structural categorization of the document base. Here, AI is to be used to support the assignment of records to SER-relevant categories, such as repository design, safety assessments, operational aspects, or regulatory documentation. The objective is not to establish definitive classifications, but to support systematic pre-structuring of large document collections and to make the underlying assignment criteria transparent and reviewable by experts.

A further use case focuses on the use of AI for targeted information retrieval and question-driven analysis. By applying predefined SER-related questions, such as whether a document contains final results, supports safety assessments, or documents key decisions, AI-supported retrieval mechanisms can be used to identify relevant document segments and highlight potentially SER-relevant content. This use case is particularly relevant for documents where the relevance cannot be reliably assessed based on title or abstract alone.

In addition, the generation of SER-oriented summaries represents another use case to be examined. Many legacy documents, especially for Konrad repository, contain abstracts or summaries of limited usefulness for SER assessment. AI-supported targeted summarization can be used to produce concise, structured summaries that explicitly reference safety-relevant content, assumptions, boundary conditions, and uncertainties, thereby improving expert access and comparability.

Finally, all these use cases together are intended to explore how the GRS approach can be operationally applied to SER-related tasks, especially for Konrad repository. They are designed to evaluate the contribution of AI to increased transparency, consistency, and reproducibility in SER identification, while clearly maintaining the role of AI as a supporting instrument within a Human-in-the-Loop framework.

2.6 AIxpertise

In 2025, GRS actively contributed to the substantive shaping and institutional positioning of the OECD-NEA initiative AIxpertise.

We coordinated GRS contributions to the Programme of Work, particularly in the areas of data, benchmarking approaches, and training, and submitted these inputs through surveys and formal feedback processes.

A key element of our engagement was our active participation in the AIxpertise Online Workshop (15–16 October 2025), which we supported technically, evaluated internally, and summarised for dissemination within GRS.

In addition, we prepared the integration of AIxpertise topics into national projects (including FLANKE-II, KISS and Doc2GraphKI) and assessed the strategic value of GRS participation.

2.7 Uncertainty and sensitivity analysis – The JOSA exercise

JOSA (Joint Sensitivity Analysis Exercise) is an international collaboration to test and investigate probabilistic sensitivity analysis methods in application to realistic numerical models in the context of radioactive waste disposal. The cooperation has been running since 2017 and so far, two reports were published /SWI 21/, /SWI 25/.

After the Volume 2 report had been published /SWI 25/, the third phase of JOSA was started. The group identified the following aspects for further investigation:

1. Nested Sampling,
2. Stochastic simulations (non-deterministic code),
3. Effects of sample type,

4. Screening methods,
5. Bifurcation effects,
6. Active Subspaces for model reduction and identification of design space,
7. Investigation of the role of input uncertainty distributions,
8. Use of input or output transformations.

In 2025, the work of GRS concentrated mainly on the Morris screening method /SWI 21/, /SWI 25/. This method is based on the effects on the model output caused by small local changes of individual parameters, called elementary effects. The mean μ of this effect (Mu) and the mean μ^* of its absolute value (Mu-Star) over the entire parameter space are estimations for global sensitivity of the parameter, assuming uniform distribution for each parameter. Moreover, standard deviation of the elementary effects (Sigma) and the bootstrapped confidence interval (Mu-Star conf) are estimated based upon the Morris samples and simulations.

The method requires a tailored sampling, so that the existing datasets could not be used for the investigation. Therefore, new datasets on the basis of Morris sampling were produced for the LILW model of GRS with 11, 15 and 20 parameters, which had been introduced in /SPI17/ and further investigated in /NOS 25/. The following questions were specifically addressed:

- How helpful is the Morris method for screening out important parameters with a low number of runs for the GRS LILW case?

- Is the Morris method capable of finding all potentially important parameters and interactions?

- Can it distinguish between “most” and “less” as well as between “less” and “almost none” significance for all parameters and interactions?

- Can the method with a larger sample size provide a clearer picture about sensitivity than with a smaller sample size?

- Is an optimised sample more suitable for the method than a standardised sample for analysing sensitivity?

2.7.1 Morris Method

The Morris method is a screening method with the goal of finding the potential few important parameters in models with many parameters with relatively small number of simulations. The ranges of the model parameter values are thereby divided into a *p*-level grid, assuming a uniform distribution for all parameters. Only for points that are part of this grid, model simulations are required. Basis of all Morris measures of sensitivity are the elementary effects (*EEs*). These effects describe the ratio of the change in model output relative to the small local variation or grid jump Δ between two input points in the parameter space.

The original or standardised Morris sample is generated by randomly selecting *j* trajectories with random starting points from the parameter space Ω. For each of these starting points, to a randomly selected input parameter x_i, a grid jump or step size Δ is added to generate a new point within Ω, i.e. $x_i + \Delta \in \Omega$. The direction of the jump or step used to generate the new point is also selected randomly. For each parameter change, the resulting *EE* is calculated. This procedure is repeated for each considered parameter. The result is a distribution of *EEs* for each model parameter. The associated computational effort is of the order of $O(j\,(n + 1))$ where *n* is the number of considered input parameters.

In mathematical terms, the elementary effect (*EE*) of the *i*-th parameter is calculated as follows:

$$EE_i = \frac{[f(x_1, x_2, \dots, x_{i-1}, x_i + \Delta, x_{i+1}, \dots, x_n) - f(x_1, x_2, \dots, x_n)}{\Delta}$$

where $y = f(x)$ is the model output function with *n* input parameters, denoted as x_i. By means of the step size $\Delta \in \{1/(p-1), 1/(p-1), \dots, 1 - 1/(p-1)\}$, the parameter space is explored where *p* represents the number of uniform grid levels to be considered. The choice of *p* and Δ depends upon the number of parameters and the possible simulation runs which can be performed. Generally, the parameter space can be better covered by the selection of a finer grid subdivision, and a smaller grid jump or step size. However, more model simulations are then required. Recommendations for the selection of *p* and Δ can be found, e.g., in /SAL 08/.

Note that when points are chosen randomly as it is done in the generation of standardised Morris samples, there is the risk that the parameter space will not be sampled as uniformly or optimal as necessary for best possible results, especially with a big number of parameters. To overcome this challenge, /CAM 07/ proposed a refined sampling strategy that allows for a better exploration of the parameter space ensuring that the resulting elementary effects yield better estimates of global sensitivity. In this strategy, from a high number of possible randomly generated trajectories, a subset of trajectories is ultimately selected which maximizes coverage of the parameter space. However, the selection of the optimal set of trajectories can be computationally expensive. To reduce the computational effort for the selection of the trajectories and with it the number of required simulations, /RUA 12/ proposed an iterative process that maximizes the distance between subgroups of generated trajectories, from which the final set of trajectories is chosen, again maximizing the distance between the different subgroups. This approach has, however, the disadvantage of not producing the optimal spread of trajectories within the parameter space.

Four Morris measures can be computed from the elementary effects *EEs*, which are the mean μ from these effects (Mu), the mean μ^* of their absolute values (Mu-Star), the standard deviation σ of these effects (Sigma) and the bootstrapped confidence interval (Mu-Star-conf). From the following formulas, Mu and Sigma can be computed:

$$\mu_i = \frac{1}{j}\sum_{r=1}^{j} EE_{i,r}$$

$$\sigma_i = \sqrt{\frac{1}{j-1}\sum_{r=1}^{j}\left(EE_{i,r} - \mu_i\right)^2}$$

Morris Mu-Star (μ^*) was introduced by /CAM 07/ to prevent classification of relevant parameters as irrelevant due to the possible cancellation of signed *EEs*. This can be the case for nonmonotonic functions. In mathematical terms, Mu-Star is calculated as follows:

$$\mu_i^* = \frac{1}{j}\sum_{r=1}^{j}\left|EE_{i,r}\right|$$

The mean measures, i.e. Mu and Mu-Star attempt to assess the change in the model output y that is expected when the parameter x_i is changed by a small step on the p grip in the parameter space. A high Mu may indicate that the parameter x_i is sensitive with respect to y. A high standard deviation (Sigma/σ) may either be a sign of interaction with other parameters and/or of nonlinearity. A small Sigma may suggest that the change in y is independent of the values of other parameters. /SAL 08/ provide the following intuitive explanation for Sigma: Under the assumption that a high Sigma value is achieved for the parameter x_i, the *EE*s would differ significantly from one another with respect to this parameter, suggesting that the value of an *EE* is strongly influenced by the choice of the sample point at which it is calculated, i.e., by the choice of values for the other parameters. In contrast, a low Sigma value implies very similar values among the *EE*s, suggesting that the effect of x_i is nearly independent of the values of the other parameters. High bootstrapping confidence interval of the Mu-Star values may indicate uncertainty about the degree of importance of the respective parameters.

In this report, the Morris method implemented in the SALib software was used, which offers generating standardised and optimised samples as well as computing the four Morris measures: Mu, Mu Star, Sigma and Mu-Star confidence interval. The generated optimised Morris samples in this report were done with the approach by /RUA 12/.

2.7.2 Description of the Test Case

The questions formulated at the beginning of Section 2.7 were addressed in some investigations using the LILW test model introduced in /SPI 17/ in variants with case 11, 15 and 20 parameters (LILW11, LILW15 and LILW20). Tab. 2.1 shows all parameters of the different LILW subcases. Tab. 2.2 lists numbers of trajectories and runs of the different LILW subcases and types of samples (standardised and optimised). 301-time steps within 10^3 to 10^6 years are analysed with Morris.

Tab. 2.1 Parameters of the of the LILW11, LILW15 and LILW20 subcases. The colours indicate the subsets of parameters that were used for the different investigations (LILW11: purple + yellow, LILW15: purple + grey, LILW20: all)

Parameter	Original type of pdf[1]	Original range or pdf parameters	Standard value	Range considered for Morris
GasEntryP: Gas entry pressure	Uniform	0 - 2.5	2.0	0 - 2.5
IniPermSeal: Initial permeability of dissolving seal	Normal	μ=-41.0605 σ=1.9809	$1.0 \cdot 10^{-18}$	μ - 2*σ - μ + 2*σ
RefConv: Reference convergence rate	Log-uniform	$1.0 \cdot 10^{-5}$ - $1.0 \cdot 10^{-4}$	$4.0 \cdot 10^{-5}$	$1.0 \cdot 10^{-5}$ - $1.0 \cdot 10^{-4}$
AEBConv: Factor of local convergence variation in AEB	Log-uniform	0.05 - 5.0	1.0	0.05 - 5.0
GasCorrPE: Organics corrosion rate	Log-normal	μ=-12.6642 σ=1.1177	$1.0 \cdot 10^{-5}$	$e^{(\mu - 2*\sigma)} - e^{(\mu + 2*\sigma)}$
TBrine: Time of brine intrusion	Log-normal	μ=8.8857 σ=0.6933	7500	$e^{(\mu - 2*\sigma)} - e^{(\mu + 2*\sigma)}$
BrineMgSat: Relative magnesium saturation of brine	Triangular	0 - 0.1 - 1.0	0.1	0 - 0.1
RGConv: Factor of local convergence variation in RG	Log-uniform	0.25 - 2.5	1.0	0.25 - 2.5
GasCorrFe: Metal corrosion rate	Log-normal	μ=-6.6728 σ=1.1177	$4.0 \cdot 10^{-3}$	$e^{(\mu - 2*\sigma)} - e^{(\mu + 2*\sigma)}$
AEBGasProd: Proportion of the material involved in gas production in AEB	Triangular	0.1 - 0.8 - 1.0	0.8	0.1 - 0.8
NABGasProd: Proportion of the material involved in gas production in NAB	Triangular	0.1 - 0.8 - 1.0	0.8	0.1 - 0.8
KonvFak: Variation factor for sheeting	Uniform	0 - 2.0	1.0	0 - 2.0
PorDebris: Porosity of debris from sheeting	Uniform	0.25 - 0.5	0.4	0.25 - 0.5

[1] Note that the pdf types are not considered in the Morris sampling

DiffCoeff: Diffusion coefficient	Log-uniform	$1.0 \cdot 10^{-10}$ - $1.0 \cdot 10^{-8}$	$1.0 \cdot 10^{-9}$	$1.0 \cdot 10^{-10}$ - $1.0 \cdot 10^{-8}$
MBConv: Factor of local convergence variation in MB	Log-uniform	0.075 - 0.75	0.2	0.075 - 0.75
RefPor: Reference porosity	Triangular	0.15 - 0.3 - 0.4	0.3	0.15 - 0.3
RGGasProd: Proportion of the material involved in gas production in RG	Triangular	0.1 - 0.8 - 1.0	0.8	0.1 - 0.8
NABConv: Factor of local convergence variation in NAB	Log-uniform	0.075 - 2.5	0.2	0.075 - 2.5
FacDisp: Longitudinal dispersion length	Triangular	0.5 - 1.0 - 2.0	0	0.5 - 1.0
C14Inv: Variation factor for C-14 inventory	Uniform	0.5 - 2.0	1.0	0.5 - 2.0

Tab. 2.2 Numbers of trajectories and runs of the different LILW subcases and types of samples

Subcase	**Typ of Sample**	**Number of Parameters**	**Number of Trajectories**	**Number of Runs**
LILW20	Standardised	20	10	210
		20	100	2100
		20	1000	21000
		20	10000	210000
	Optimised (Opt)	20	10	210
		20	100	2100
LILW15	Standardised	15	10	160
		15	100	1600
		15	1000	16000
		15	10000	160000
LILW11	Standardised	11	10	120
		11	100	1200
		11	1000	12000
		11	10000	120000

2.7.3 Results

2.7.3.1 Results with Standardised Samples

Morris Mu-Star Results: For the LILW20 subcase, with the small standardised Morris sample with 10 trajectories, big outliers of Morris Mu-Star of, e.g., the parameters IniPermSeal, RefConv and GasCorrFe are produced for certain time periods, see Fig. 2.5. Fig. 2.5 presents Mu-Star results of the LILW20 subcase with all samples plotted versus time from 10^3 to 10^6 years. The sample with 100 trajectories also seems still to generate bumps in the time curves and/or outliers of Mu-Star like for BrineMgSat. With this kind of bumps, this parameter appears to be important for the LILW20 subcase. However, results with higher sample sizes indicate that BrineMgSat is less important. The Mu-Star values converge pretty well with the two largest samples with 1000 and 10000 trajectories. Though, the time curve with 1000 trajectories has still bumps, see Fig. 2.5 and Fig. 2.6. Fig. 2.6 shows Mu-Star results versus time with the focus on the less important parameters of the LILW20 subcase with the samples with 1000 and 10000 trajectories. Thus, potential outliers and bumps in the Mu-Star results can apparently be minimised with a sample of larger size associated with a better coverage of the parameter space. Results are then also more robust and would make classification of the parameters clearer.

According to Mu-Star using the largest samples, it appears that the following five parameters are important for certain time periods: IniPermSeal, TBrine, AEBConv, and RefConv, and GasEntryP, see Fig. 2.5, and the following five are less significant for the LILW20 subcase: RGConv, GasCorrPE, BrineMgSat, AEBGasProd and GasCorrFe, see Fig. 2.6. The parameters KonvFak, PorDebris, DiffCoeff, MBConv and RefPor also show some Mu-Star with the largest samples with 1000 and 10000 trajectories, see Fig. 2.6. Other methods of sensitivity analysis, however, do not identify these parameters as important. One has to keep in mind, though, that these other methods, unlike Morris, take account of the original distributions (see Tab. 2.1), which normally give lower weight to extreme values than a uniform distribution. The five parameters C14Inv, NABConv, RGGasProd, NABGasProd and FacDisp show nearly no Mu-Star with the big samples.

There is also a trend in the LILW15 Mu-Star results as in the LILW20 results, that the parameters KonvFak and RefPor are less important for certain time periods, see Fig. 2.7. Fig. 2.7 presents Mu-Star results of the LILW15 subcase versus time with all samples. There is nearly no Mu-Star for the three parameters PorDebris, DiffCoeff and

MBConv which indicates no importance of these parameters. The LILW20 subcase, according to Mu-Star, indicated less significance of these parameters, see above. The Mu-Star results of the LILW15 subcase with 1000 and 10000 trajectories (16000 and 160000 runs) confirm the findings of the LILW20 subcase that IniPermSeal, TBrine, AEBConv, GasEntryP and RefConv are important parameters and BrineMgSat, GasCorrPE, RGConv, AEBGasProd and GasCorrFe are less important parameters. To prevent big outliers and/or bumps in the Mu-Star results for the LILW15 subcase, the lowest sample sizes with 10 and 100 trajectories (160 and 1600 runs) for a standardised sample are too small. For example, some striking peaks or outliers appear in the results for otherwise (less) important parameters with the smallest samples; e. g. for parameters BrineMgSat, GasEntryP and IniPermSeal. An interesting behaviour shows the parameter TBrine. It does not appear important with a low sample size with 10 trajectories for the LILW15 subcase. With the next largest sample with 100 trajectories (1600 runs) for this subcase, TBrine seems less important and with trajectories of 1000 and 10000 (16000 and 160000 runs), it appears important. The Mu-Star of the LILW20 subcase with all sample sizes indicated that TBrine is important.

Similar to LILW20 and LILW15, the Mu-Star results for the LILW11 subcase indicate that the parameters IniPermSeal, TBrine, AEBConv, GasEntryP and RefConv are important, while BrineMgSat, GasCorrPE, RGConv, AEBGasProd and GasCorrFe are less important for certain time periods, see Fig. 2.8. Fig. 2.8 demonstrates Mu-Star results of the LILW11 subcase versus time with all samples. For NABGasProd, Mu-Star is nearly zero. Samples with 1000 trajectories (12000 runs) seem to be suitable for getting smoother Mu-Star results. Like for the LILW20 and LILW15 subcases, a standardised sample with 10 trajectories (120 runs) appears too small for reliable results. Conspicuous outliers of Mu-Star for the LILW11 subcase with this sample size are visible in the time curves for the less important parameters RGConv and GasCorrFe and the important parameters RefConv, TBrine, GasEntryP and IniPermSeal.

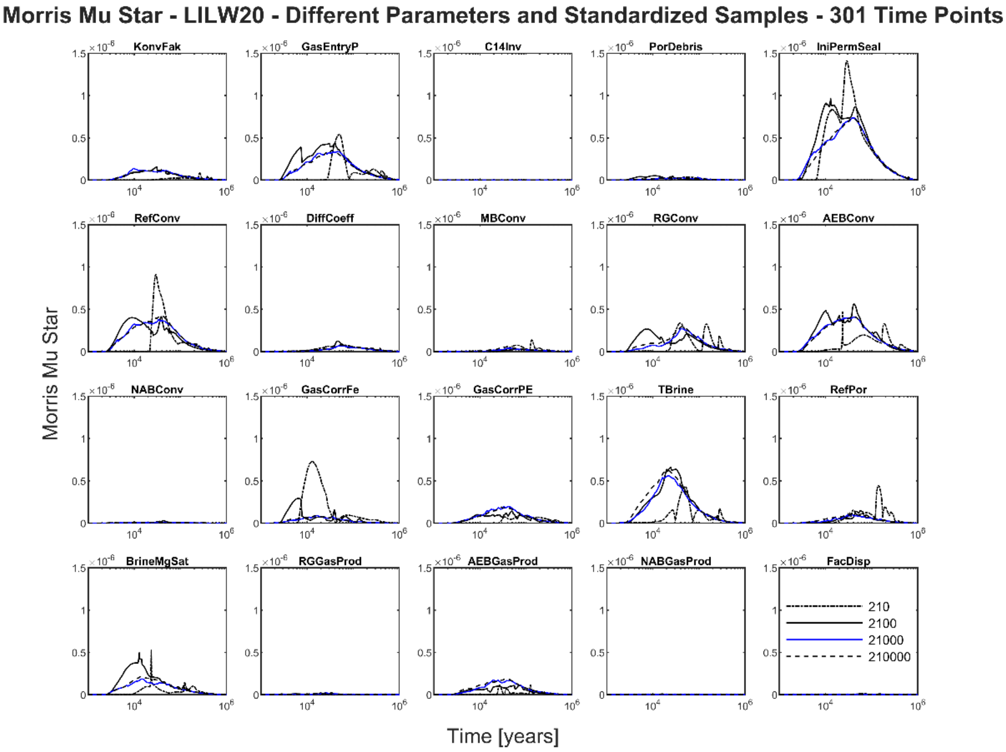

Fig. 2.5 Mu-Star of LILW20 versus time for all parameters with all standardised samples

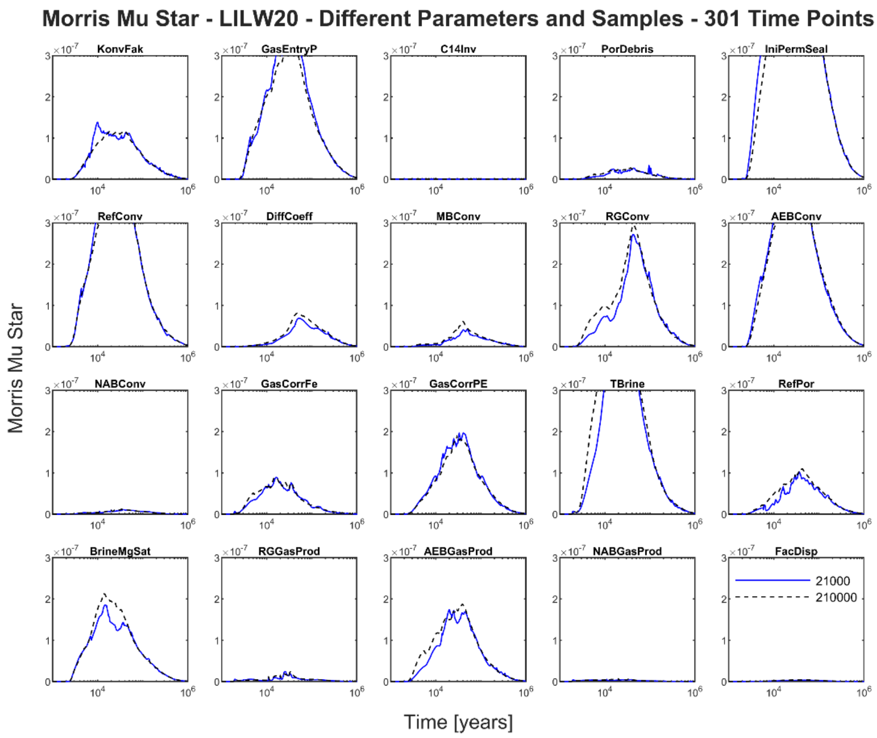

Fig. 2.6 Mu-Star of LILW20 versus time with the focus on the less important parameters with the largest samples with 1000 and 10000 trajectories

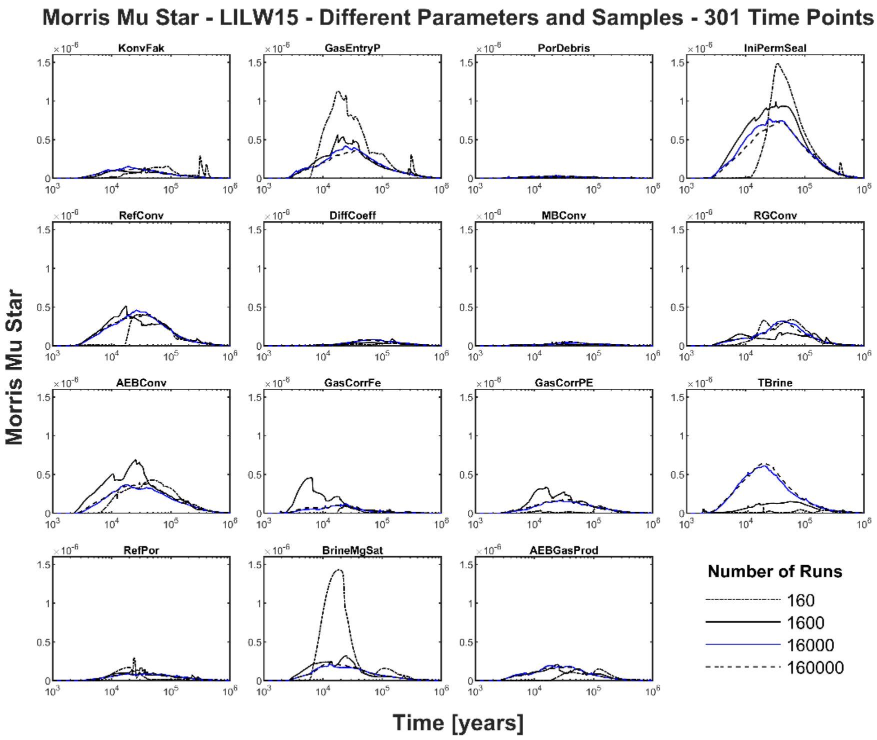

Fig. 2.7 Mu-Star of LILW15 versus time for all parameters with all samples

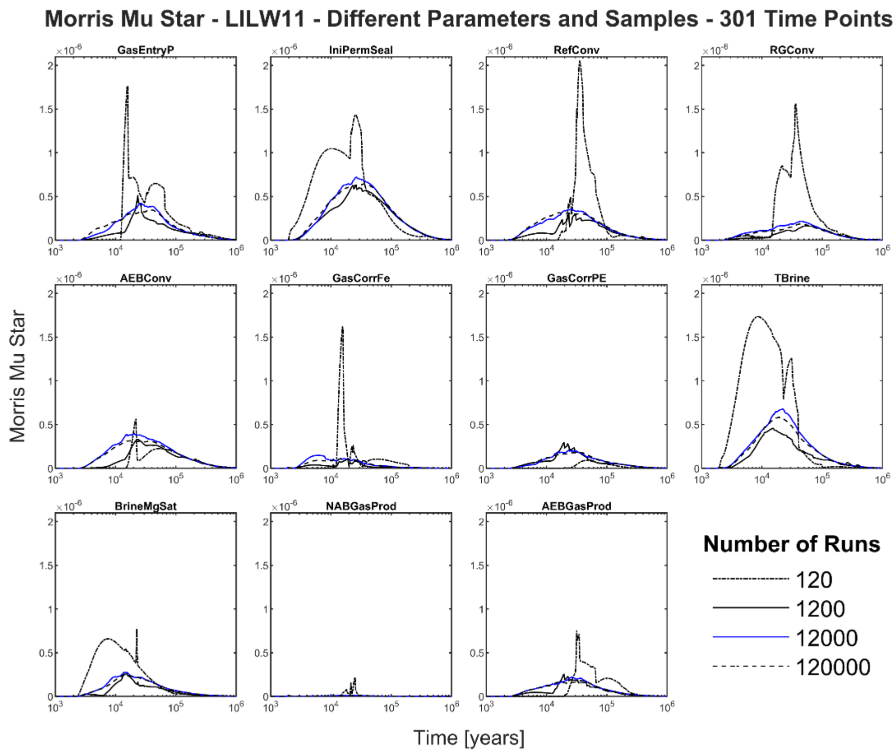

Fig. 2.8 Mu-Star of LILW11 versus time for all parameters with all samples

Morris Mu Results: For the LILW20 results, smooth and converging Mu results are obtained with a standardised sample starting from 1000 trajectories (21000 runs), see Fig. 2.9. Fig. 2.9 presents Mu versus time for the LILW20 subcase with all samples. For this subcase, especially with the lowest sample with 10 trajectories (210 runs), negative Mu values occur for some of the parameters like GasCorrFe, RefConv, AEBConv and RefPor, where high sample sizes lead to clearly positive values and/or much smaller negative Mu values. Moreover, positive values of Mu are produced for TBrine with the lowest sample while with the higher samples, TBrine has only negative Mu values. This observation confirms that, at least in this case, 10 trajectories are too few to yield reliable Mu measures. Mu values with 100 trajectories seem to be more reliable but the different irregularities create challenges in classification of the parameters. An example for this is the parameter BrineMgSat as it was for Mu-Star. With 100 trajectories, this parameter appears important but with 1000 and 10000 trajectories, only less important.

Unlike Mu-Star, Mu is a signed sensitivity measure. A negative Mu value means that negative elementary effects dominate, but it does not mean that increase of the parameter leads, under all circumstances, to decrease the model output. The behaviour can be influenced by other parameters. A near-zero Mu can be a sign for generally low parameter relevance, but it can also indicate an uneven model behaviour.

For the LILW20 subcase, IniPermSeal has the biggest Mu values and TBrine shows the most conspicuous negative Mu, see Fig. 2.9: RGConv exhibits a change from positive to negative Mu, see Fig. 2.10. Fig. 2.10 shows Mu results versus time with the focus on the less important parameters of the LILW20 subcase with the samples with only 1000 and 10000 trajectories. For the six potential less important parameters from the Mu-Star analysis, PorDebris, DiffCoeff, MBConv, RefPor, GasCorrFe and KonvFak, using the samples with 1000 and 10000 trajectories (21000 and 210000 simulations), near-zero Mu values are calculated, see Fig. 2.10. This contrasts with the Mu-Star results for this subcase. Mu-Star sums up the absolute values, which may help identify additional important parameters.

Mu results from all subcases with largest samples confirm all important parameters found by Mu-Star, i.e., IniPermSeal, TBrine, AEBConv, GasEntryP and RefConv and the four less important parameters BrineMgSat, GasCorrPE, RGConv, AEBGasProd, see Fig. 2.10 to Fig. 2.12. In contrast to LILW20 and of LILW15, Mu of the LILW11 subcase indicates that GasCorrFe may be a less important parameter with 1000 and 10000 trajectories (12000 and 120000 simulations) with non-monotonic behaviour, see Fig. 2.12. The

Mu-Star results for all subcases indicated less importance of this parameter. Fig. 2.11 and Fig. 2.12 present Mu versus time for the LILW15 and LILW11 subcases with all samples, respectively.

For the LILW15 subcase, as for the LILW20 case, there is also nearly no Mu for the four parameters PorDebris, DiffCoeff, MBConv and RefPor with 1000 and 10000 trajectories. There is a little more Mu for KonvFak and GasCorrFe, see Fig. 2.11. It is questionable, however, whether this little bit is enough to assign a certain importance.

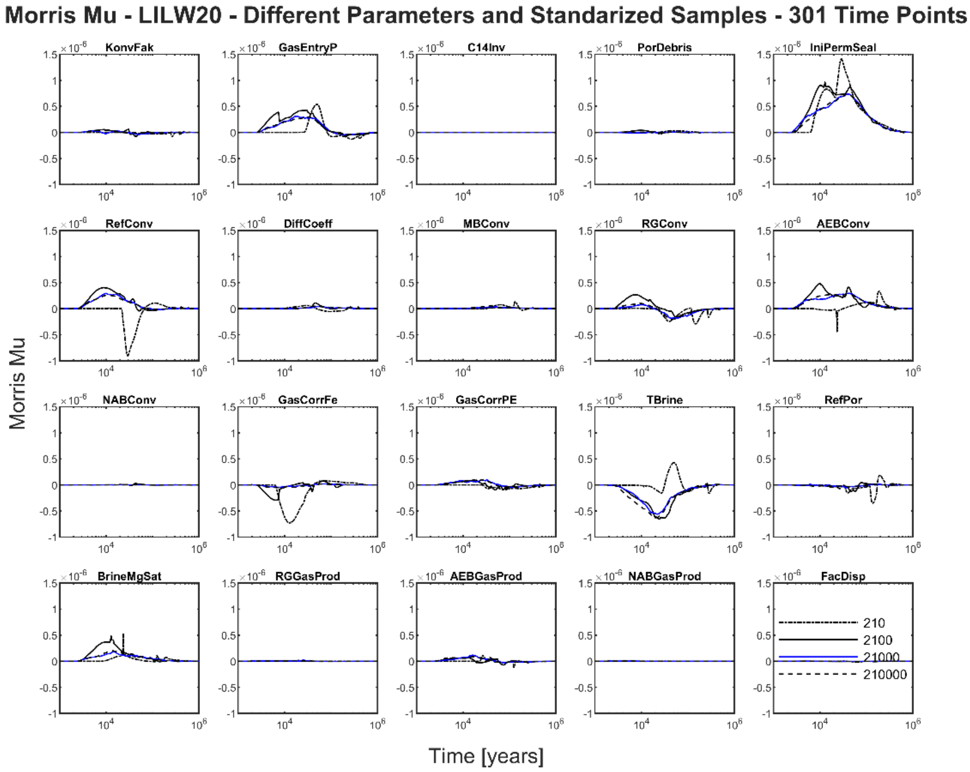

Fig. 2.9 Mu of LILW20 versus time for all parameters with all standardised samples

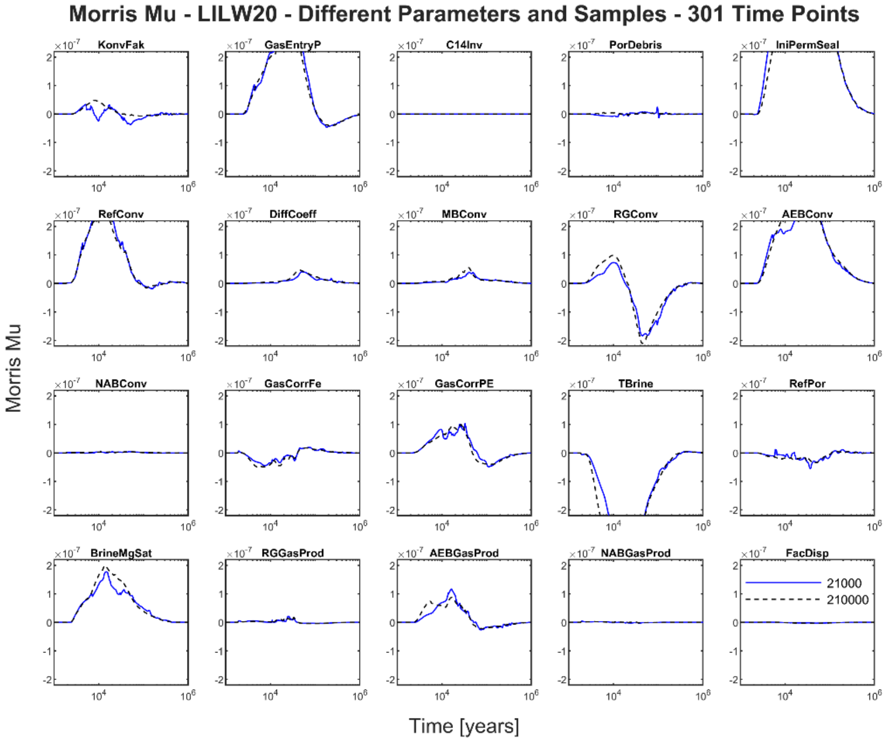

Fig. 2.10 Mu of LILW20 versus time with the focus at the less important parameters with the largest samples

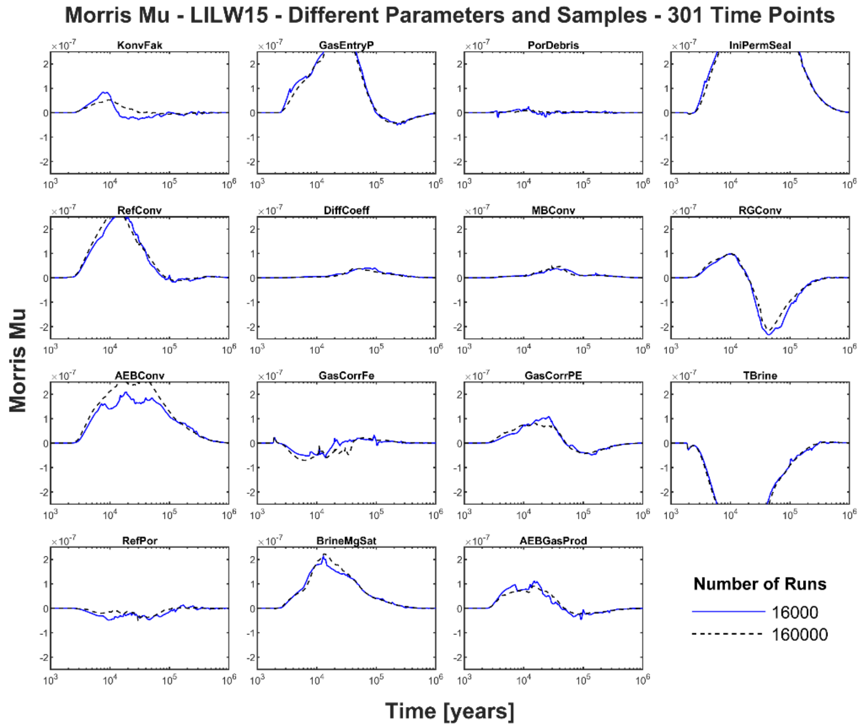

Fig. 2.11 Mu of LILW15 versus time with the focus at the less important parameters with the largest samples

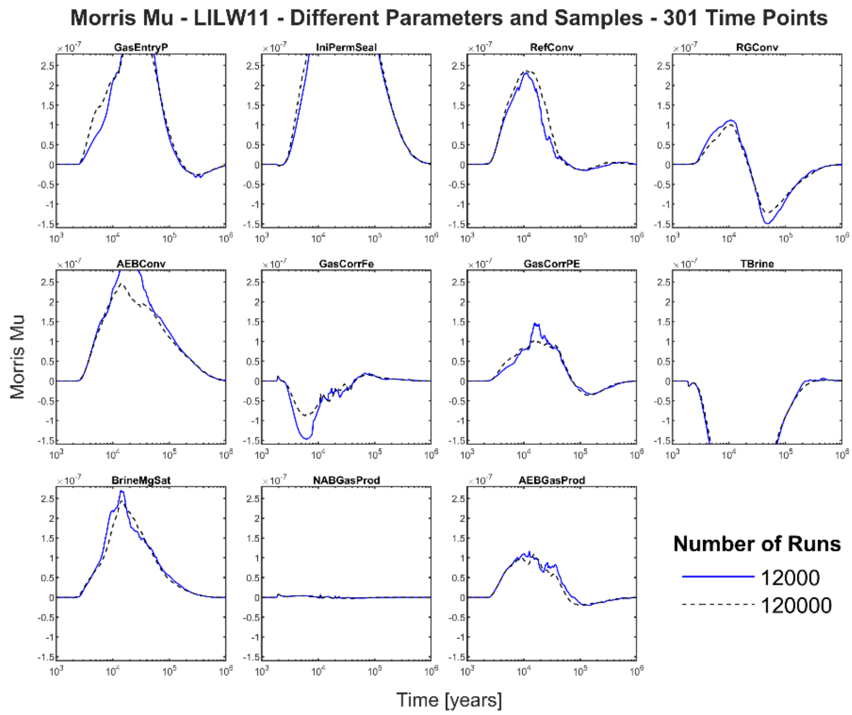

Fig. 2.12 Mu of LILW11 versus time with the focus at the less important parameters with the largest samples

Morris Sigma Results: For all LILW subcases, according to the magnitude of the Sigma values, with a high number of trajectories, all important and less important parameters according to the Mu-Star analysis seem to have interactions (see Section 2.7.1) with other parameters which are IniPermSeal, AEBConv, GasEntryP, TBrine, RefConv, BrineMgSat, RGConv, GasCorrPE, AEBGasProd and GasCorrFe, see Fig. 2.13 to Fig. 2.16. Fig. 2.13 shows Sigma values of LILW20 subcase with all standardised samples while Fig. 2.14, Fig. 2.15 and Fig. 2.16 only demonstrate Sigma values of the LILW20, LILW15 and LILW11 subcases with the two largest samples, respectively. For the LILW20 subcase, there is nearly no Sigma for NABGasProd, NABConv, C14Inv and FacDisp, which indicates that these parameters do not interact with other parameters. Also, the Sigma values of PorDebris, DiffCoeff, MBConv and RGGasProd for this sub-case are very low. For the LILW15 subcase, PorDebris, DiffCoeff and MBConv have also small Sigma values with 1000 and 10000 trajectories, see Fig. 2.15.

For the LILW20 and LILW15 subcases, the potentially less important parameters KonFak and RefPor according to the Mu-Star analysis have a rather big Sigma with 1000 and 10000 trajectories, see Fig. 2.14 and Fig. 2.15. This might be an indication for significant interactions of these parameters with others, but the Morris method does not allow a reliable interpretation of such results.

For all LILW subcases, there are some bumps in the Sigma results even with largest samples, i.e. with 1000 and 10000 trajectories. Fig. 2.13 demonstrates Sigma values of LILW20 versus time where the outliers and bumps in the time curves for all samples are shown.

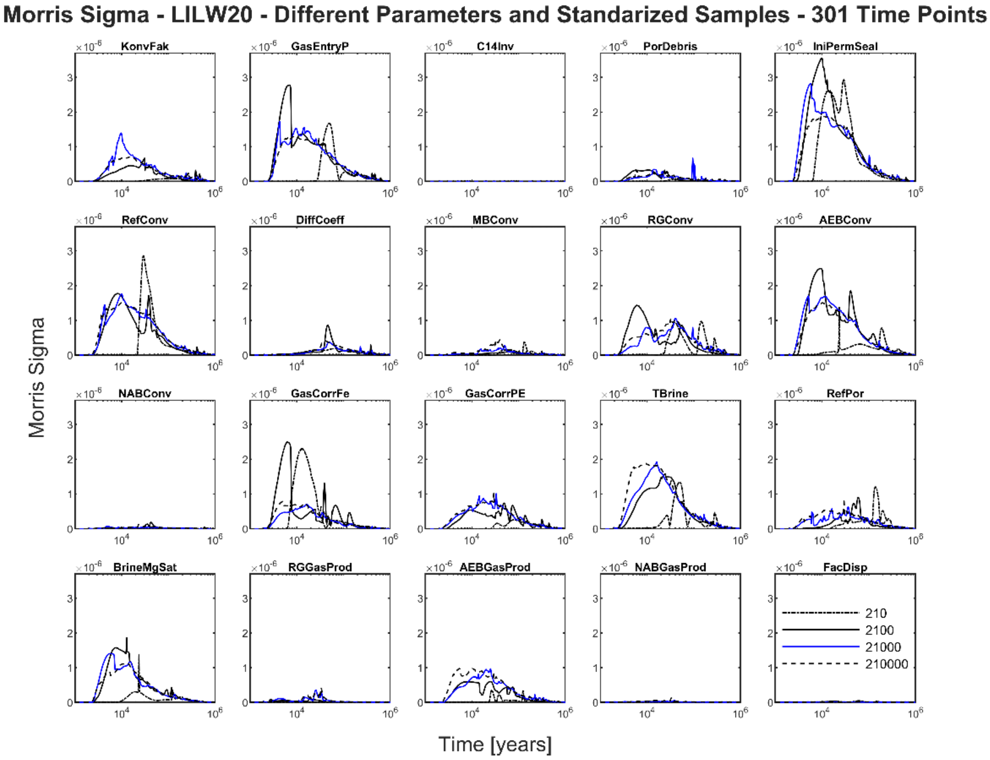

Fig. 2.13 Sigma of LILW20 versus time for all parameters with all standardised samples

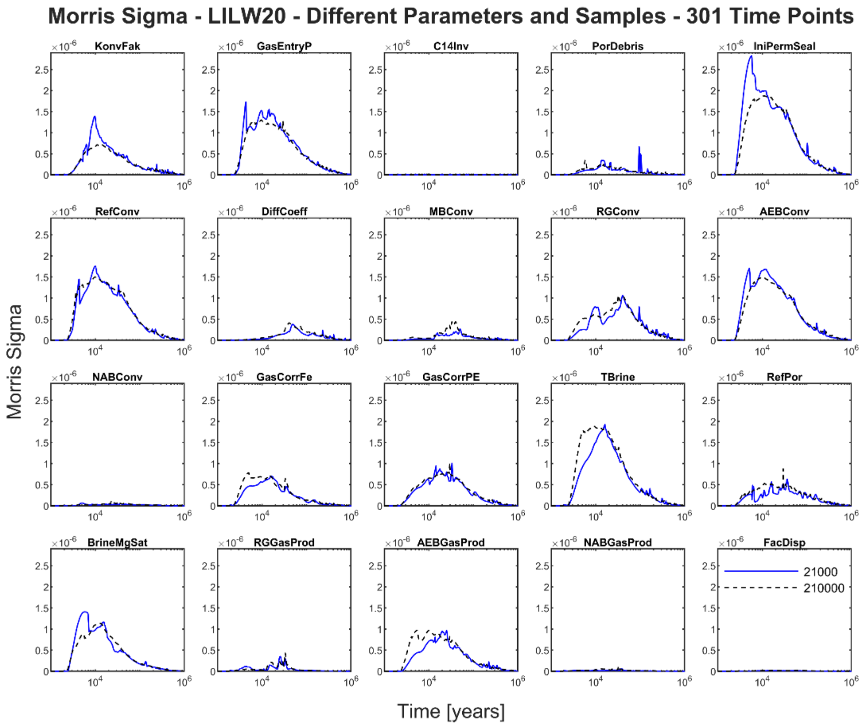

Fig. 2.14 Sigma of LILW20 versus time with the focus at the less important parameters with the largest samples

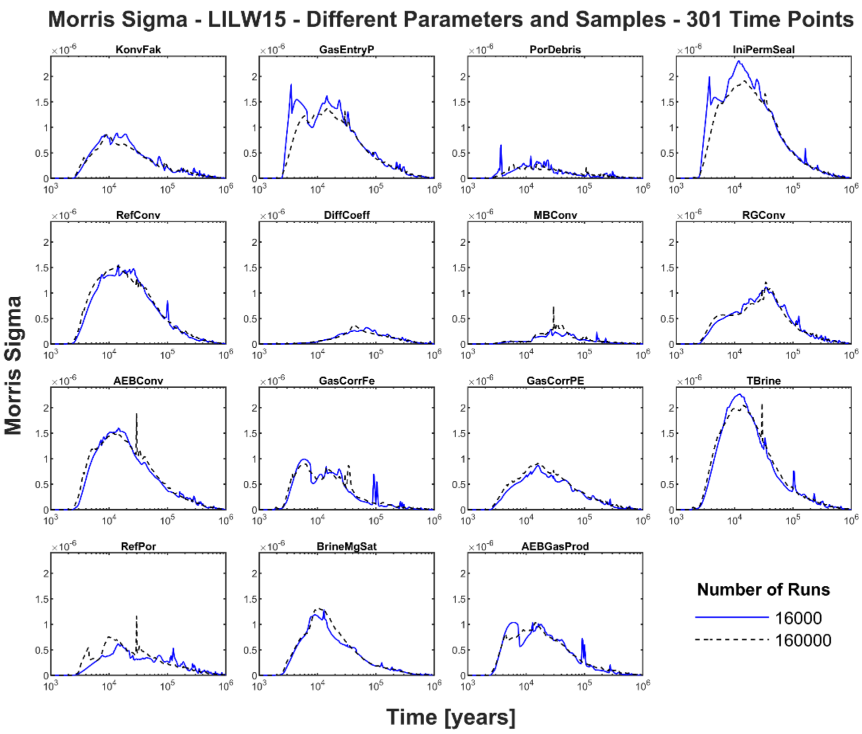

Fig. 2.15 Sigma of LILW15 versus time with the focus at the less important parameters with the largest samples

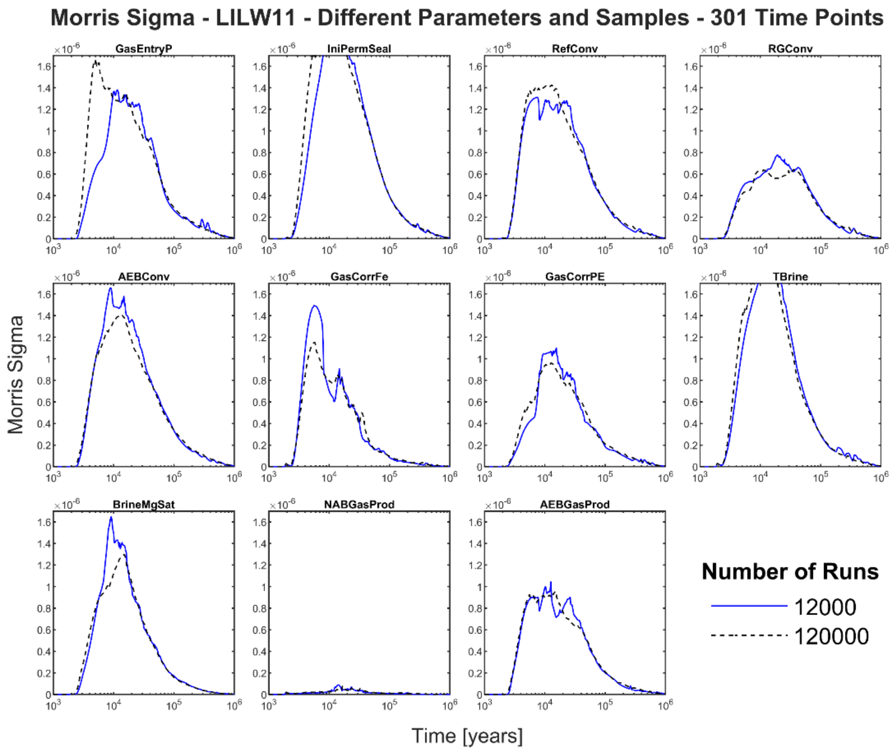

Fig. 2.16 Sigma of LILW11 versus time with the focus at the less important parameters with the largest samples

Morris Mu-Star Confidence Interval Results (Bootstrapped Confidence Interval): For the LILW20 and LILW15 subcases, the three parameters KonFak, RefPor and GasCorrFe, which are less important according to the Mu-Star analysis, have a rather big Mu-Star Conf with 1000 and 10000 trajectories, see Fig. 2.17 and Fig. 2.18. This might be a hint to higher order effects by parameter interactions, but such results are difficult to interpret. The other less important parameters PorDebris, DiffCoeff and MBConv have a smaller Mu-Star Conf than those mentioned above. GasCorrFe has also a considerable Mu-Star Conf, especially for the LILW11 subcase with 1000 and 10000 trajectories, see Fig. 2.19. Fig. 2.17, Fig. 2.18 and Fig. 2.19 present the bootstrapping confidence interval versus time for all parameters with the largest samples of the LILW20, LILW15 and LILW11 subcases, respectively. The decrease of bootstrapping confidence interval for all parameters with higher numbers of trajectories confirms some uncertainty due to poor coverage of the parameter space. The bumps are even more pronounced in the bootstrapping confidence interval with largest samples than in the Sigma results.

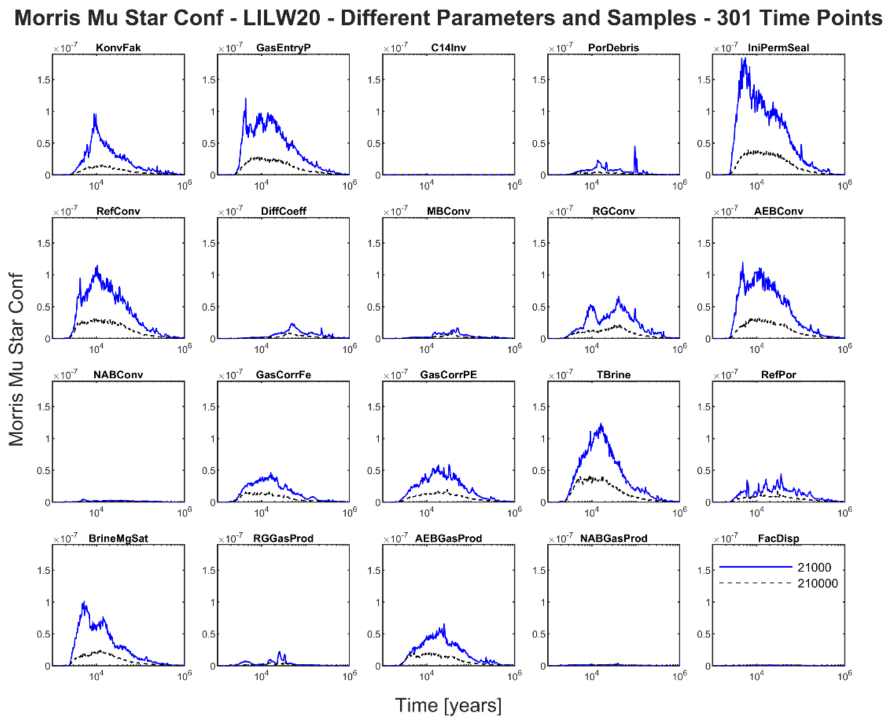

Fig. 2.17 Morris bootstrapping interval of LILW20 versus time for all parameters with the largest samples

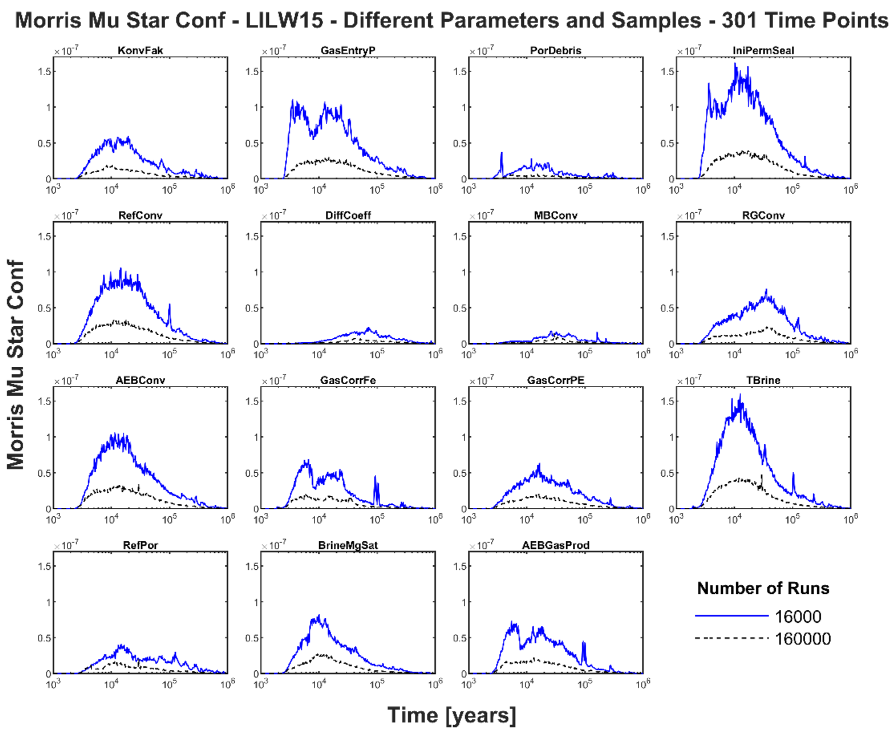

Fig. 2.18 Morris bootstrapping interval of LILW15 versus time for all parameters with the largest samples

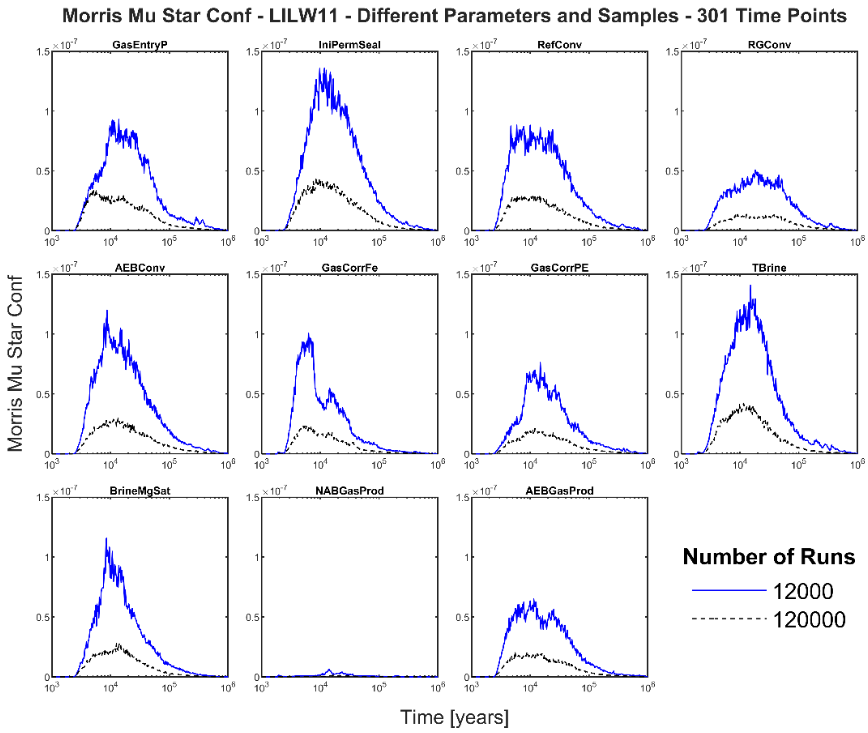

Fig. 2.19 Morris bootstrapping interval of LILW11 versus time for all parameters with the largest samples

2.7.3.2 Results with Optimised Samples

It appears that there is a certain improvement in results with optimised samples. Assuming that the investigations with standardised samples of 1000 and 10000 trajectories are close to the "truth", optimised samples of 10 or 100 trajectories produce more reliable Morris results than with standardised samples of same size, especially with the ones with 100 trajectories, see Fig. 2.20 to Fig. 2.23. Fig. 2.20 to Fig. 2.23 demonstrate Mu-Star, Mu, Sigma and Mu-Star Conf versus time with the optimised samples with 10 and 100 trajectories in comparison to the ones with the standardised samples with 1000 and 10000 trajectories. However, classification of the parameters with the optimised samples do not quite agree with those with the standardised samples with 1000 and 10000 trajectories. For example, Mu-Star and Mu of AEBConv with optimised sample with 100 trajectories appear less important and not important as with Mu-Star and Mu using the standardised samples with 1000 and 10000 trajectories. There seem to be outliers of Mu-Star, Mu and Sigma of e.g., RefPor, RefConv, BrineMgSat, TBrine and AEBConv with optimised sample with 10 trajectories, see Fig. 2.20, Fig. 2.21 and Fig. 2.22. In addition, there are still bumps in the time curves of the different Morris measures using the optimised sample with 100 trajectories. Mu-Star conf is for some parameters higher with optimised samples, like for RefConv with 100 trajectories and for some lower like for AEBConv with 100 trajectories in comparison with the ones with standardised samples with 1000 and 10000 trajectories, see Fig. 2.23. Consequently, it also appears as with standardised sampling that for the optimised sampling strategy after /RUA 12/ more than 100 trajectories are required to obtain a reliable classification of the parameters with regards to their degree of importance. Maybe, for the optimised sampling strategy after /RUA 12/, 200 trajectories are sufficient for a reliable classification of the parameters. This seems much better than with standardised samples, but the required number of runs are still too high for usage of the Morris method. A realistic number of trajectories for a sampling strategy for Morris screening may be in the range of ten to one hundred to keep number of required runs in a reasonable order of magnitude. But this in general depends strongly upon e.g., considered model, computational effort and number of parameters. The optimised sampling strategy after /CAM 07/ may provide better results with trajectories between 10 and 100. Though, finding the optimal trajectories from a high number of trajectories may be computational expensive.

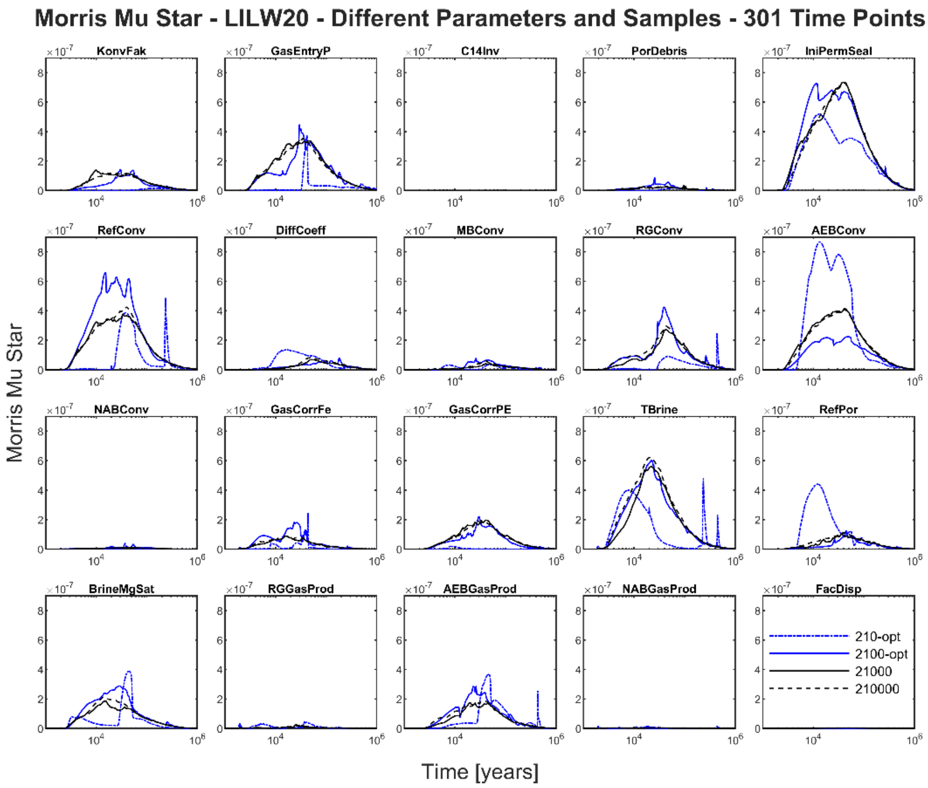

Fig. 2.20 Mu-Star of LILW20 versus time for all parameters with optimised samples in the sizes of 210 and 2100 runs compared to the ones with standardised samples with 21000 and 210000 runs

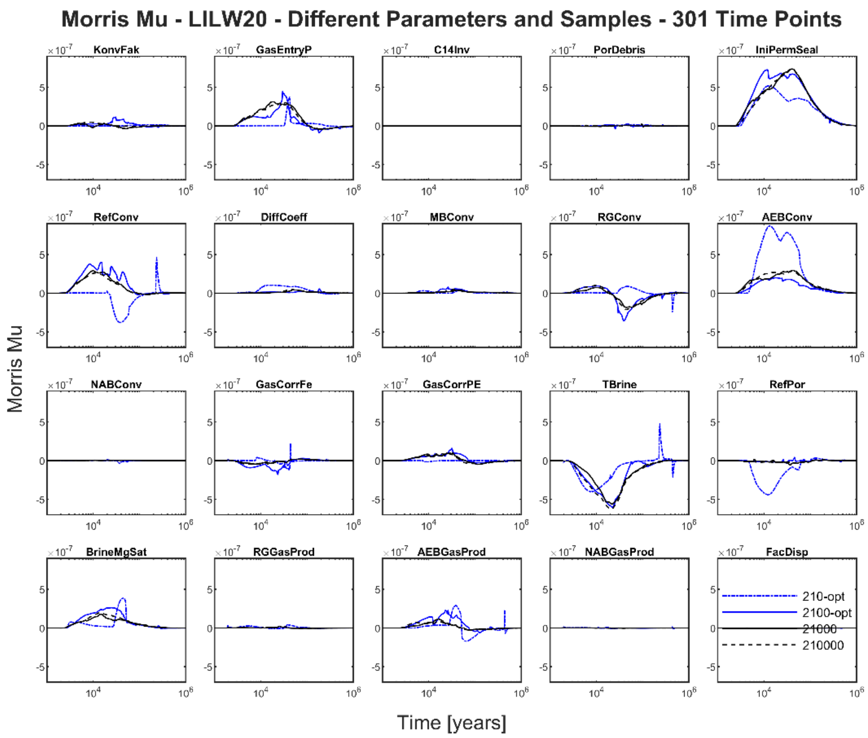

Fig. 2.21 Mu-of LILW20 versus time for all parameters with optimised samples in the sizes of 210 and 2100 runs compared to the ones with standardised samples with 21000 and 210000 runs

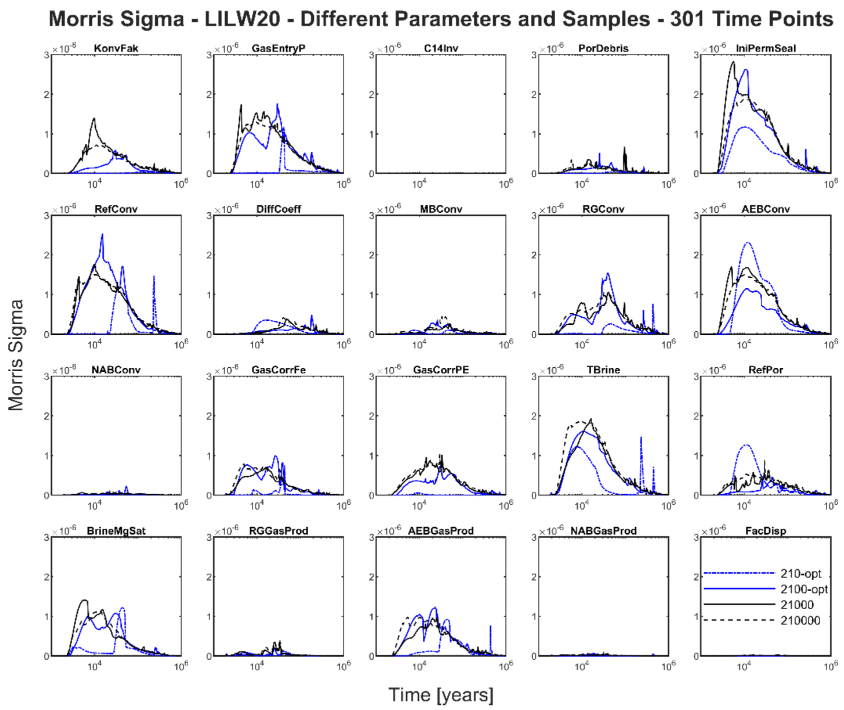

Fig. 2.22 Sigma-of LILW20 versus time for all parameters with optimised samples in the sizes of 210 and 2100 runs compared to the ones with standardised samples with 21000 and 210000 runs

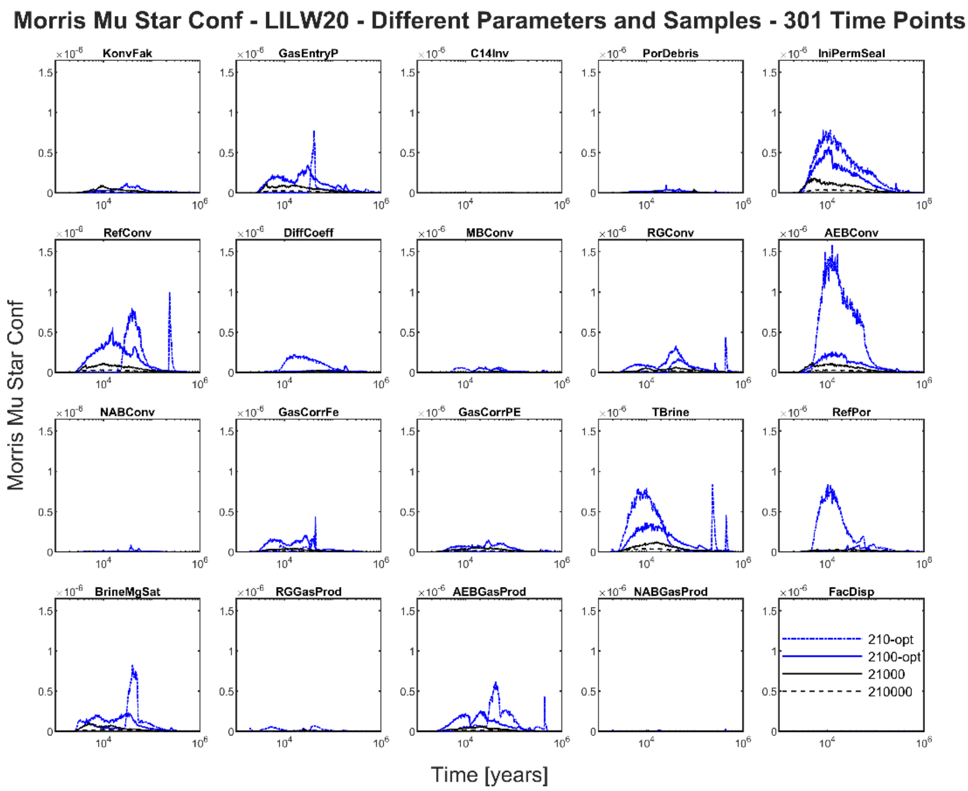

Fig. 2.23 Mu-Star conf-of LILW20 versus time for all parameters with optimised samples in the sizes of 210 and 2100 runs compared to the ones with standardised samples with 21000 and 210000 runs

2.7.4 Summary

The JOSA case „GRS LILW" was investigated with the screening method by Morris. This case was investigated in form of three subcases, considering 11, 15 and 20 parameters, i.e. LILW11, LILW15 and LILW20, respectively, to answer as best as possible the questions mentioned in Section 2.7. The following sample sizes were used for the subcases with the different numbers of varying parameters:

- LILW11: four standardised samples with 10, 100, 1000 and 10000 trajectories, in sizes of 120, 1200, 12000 and 120000 runs, respectively

- LILW15: four standardised samples with 10, 100, 1000 and 10000 trajectories, in sizes of 160, 1600, 16000 and 160000 runs, respectively

- LILW20: four standardised samples with 10, 100, 1000 and 10000 trajectories, in sizes of 210, 2100, 21000 and 210000 runs, respectively and two optimised samples with 10 and 100 trajectories in sizes of 210 and 2100 runs.

Results were analysed via mean elementary effects (Mu), mean of absolute values (Mu-Star), standard deviation of the elementary effects (Sigma) and bootstrapped confidence interval (Mu-Star conf) with 301-time steps within the time period from 10^3 to 10^6 years.

For all subcases, it seems that a first screening of potential important parameters can already be done with a small, standardised Morris sample with 100 trajectories, but not necessarily a classification of the parameters as most important, less important or (nearly) unimportant, or a parameter ranking, as the Morris measures are often far from convergence in comparison to the ones using a sample of higher sizes. With this sample size there are still some bumps in the time curves and/or outliers of the Morris measures, which make classification of the parameters additionally challenging. For example, BrineMgSat has bumps in the Mu-Star and Mu results for the LILW20 case over a certain time period with a sample size with 100 trajectories, which gives the impression that BrineMgSat is an important parameter. However, Mu-Star and Mu results with higher sample sizes indicate that BrineMgSat is less important. With the smallest, standardised Morris sample with only 10 trajectories, conspicuous outliers of the Morris measures and bumps in the time curves were produced for some parameters and certain time periods. Challenges in convergence of the Mu-Star and Mu results with too low sample size can occur as demonstrated, for instance, by the LILW15 subcase with the parameter TBrine. With the sample with only 10 trajectories, it was indicated as not important, with 100 trajectories, less important and with 1000 and 10000 trajectories important. Outliers and bumps or irregularities in the results can apparently be minimized using larger samples to better cover the parameter space. Moreover, some relative high negative Morris Mu appeared particularly with the lowest sample size with 10 trajectories, for example of the LILW20 subcase for the parameters GasCorrFe, RefConv, AEBConv and RefPor, where high sample sizes lead to clearly positive values and/or much smaller negative Mu values. In addition, for the LILW20 subcase, positive values of Mu are produced for TBrine with the lowest sample while with the higher samples, TBrine has only negative Mu values. This observation confirms that, at least in this case, 10 trajectories are too few to yield reliable Mu measures. The bootstrapped confidence intervals often shrink with increasing sample size, which is also a sign for more robustness of the results.

The following five parameters for all subcases appear to be important according to Mu-Star and Mu: IniPermSeal, TBrine, AEBConv, GasEntryP and RefConv and the following four as less significant for all subcases: RGConv, GasCorrPE, BrineMgSat and AEBGasProd. Mu-Star indicated GasCorrFe for all subcases as less important and Mu only for the LILW11 subcase. For all just mentioned important and less important parameters, Morris Sigma indicates some parameter interactions and/or nonlinearity for these. There are some bumps in the Sigma results also with largest samples, i.e. with 1000 and 10000 trajectories. The bumps are even bigger in the bootstrapping confidence intervals.

Mu-Star of the LILW20 case indicated, even with 1000 and 10000 trajectories, that there may be five further less important parameters, which are KonvFak, PorDebris, DiffCoeff, MBConv and RefPor. So far, other methods of sensitivity analysis have not indicated these with any degree of significance. The comparability is limited, however, since the Morris method disregards the original distributions and assumes uniformly distributed values for all parameters within their possible intervals. The Mu results of the LILW20 subcase with big sample sizes, i.e. 1000 and 10000 trajectories (21000 and 210000 runs) tend to show that these parameters are not important. Mu-Star sums up all absolute values, so that, in contrast to Mu, random positive and negative deviations do not cancel each other out, which may help identify additional important parameters. In the LILW20 and LILW15 subcase, the parameters KonvFak and RefPor show larger Sigma and Mu-Star conf than expected. This might be an indication for significant interactions of these parameters with others, but the Morris method does not allow a reliable interpretation of such results.

Mu-Star and Mu of the LILW15 case with the biggest samples also indicate KonvFak and RefPor as less important parameters but not PorDebris, DiffCoeff and MBConv, with the exception that Mu tends to show that RefPor is not important.

TBrine showed the most distinct negative effect, RGConv and GasCorrFe exhibit a change of sign during the simulation period for all subcases.

The optimised sampling approach after /RUA 12/ used in this report appeared to improve results, especially with the highest considered sample size with 100 trajectories. However, these results do not seem quite reliable for the classification of the parameters. A good example for this is AEBConv which Mu-Star and Mu showed up as less important with 100 trajectories. The standardised samples for all subcases in particular with highest number of runs, Mu-Star and Mu indicated AEBConv as an important parameter. For some of the parameters like for RefPor, RefConv, BrineMgSat, TBrine and AEBConv, there are still outliers of Mu-Star, Mu and Sigma with optimised sample with 10 trajectories. In addition, there are still bumps in the time curves of the different Morris measures using the optimised sample with 100 trajectories. Mu-Star conf is for some parameters higher with optimised samples, like for RefConv with 100 trajectories and for some lower like for AEBConv with 100 trajectories in comparison with the ones with standardised samples with 1000 and 10000 trajectories. The results with optimised sample with 100 trajectories gave the impression that 1000 trajectories are not necessary as for the standardised sample to obtain converging time curves. Maybe 200 trajectories are already sufficient for the optimised sampling approach after /RUA 12/.

In summary, results of the GRS LILW case indicate that for a complex case, big sizes of samples with at least 1000 trajectories for the standardised approach and/or better structured Morris samples are required to minimize outliers and bumps in the results of the Morris measures of sensitivity. Outliers and bumps in the results of the Morris measures of sensitivity make it very difficult to classify parameters as most important, less important, or (nearly) unimportant. The LILW case shows complex behaviour including quasi-discrete behaviour, which can cause some jumps in the model output values.

2.7.5 Conclusions

The Morris method seems to be suitable for finding all potentially important parameters and interactions with relatively small numbers of runs. However, it appears that there are challenges with classifying some parameters and interactions as “most” or “less” important as well as “less” or “nearly not” important. Therefore, the set of potentially important parameters may include some parameters which finally turn out to be not important. The Morris method is not appropriate to classify all degrees of significance of the different parameters and interactions as it was designed as a screening method and not a quantifying method like variance-based sensitivity analysis. After all, it is a big advantage with Morris to be able to reduce the number of parameters for further in-depth analysis like with variance-based or other methods.

For a better classification of significant and less significant parameters, the selection of appropriate sample sizes and analysis with more than one sample size are helpful as they support analysis of convergence of the sensitivity measure and may avoid as far as possible outliers or numerical artifacts of the Morris sensitivity measures as well as misleading Mu values of some parameters with too low sample sizes and large bootstrapping convergence intervals. The classification of the parameters as less or not important appears to be even more challenging with Morris. Even large samples may not provide a clear picture about this. Though, it is unpractical using large samples with 1000 or more trajectories for the Morris method, as these require many model evaluations that cannot be re-used for other investigations. A guideline for a number of trajectories may be between 10 and 100 but this range depends strongly upon investigated case and its computational costs. A first screening with the Morris method is useful. After that it may be much better using different methods of sensitivity analysis for the classification and ranking of the parameters. In addition, it may be supportive confirming classification of the parameters and interactions by investigating the case with different number of parameters as it was done in this report.

With optimised sampling approach after /RUA 12/, comparably reliable results to a standardised sample with 1000 trajectories may be obtained with a reduced number of trajectories, maybe with 200 trajectories. An optimised sample after /CAM 07/ with optimised spread in the realistic range of trajectories between 10 and 100 may be another alternative to further improve results associated due to better coverage of the parameter space. The approach after /RUA 12/ for the generation of an optimal sample has the advantage of reducing the computational effect when the number of parameters is high, but it has the disadvantage of not producing the most optimal spread of trajectories within the parameter space. The approach after /CAM 07/ may provide better results in the realistic range of trajectories but it may be computational more expensive finding the optimal trajectories in the parameter space.

2.8 EBS Task Force

The Task Force on Engineered Barriers initiated by SKB was terminated at the end of the year 2025. Until then, Task 14a based on experimental data obtained from the project WiGru-7 /NOS 18/ was led by GRS. The primary objective of this task was to investigate the capability of different modelling approaches to reproduce the experimentally observed hydraulic behavior of compacted bentonite at limited water supply. All in all, parties from Sweden, Japan, Czech Republic and Germany took actively part in Task 14a. All other participants of the Task Force EBS gave advice and support to the Task leader (GRS).

2.8.1 Experimental Setup

The experiment was concerned with mechanically confined samples of MX-80 bentonite with an air-dry density of 1450kg/m³. The cylindrical specimen had a diameter of 50 mm and a length of 40 mm. Mechanical confinement was maintained throughout the experiment in order to simulate conditions relevant for engineered barrier systems in deep geological repositories.

Water supply was provided from the bottom of the sample. The inflow was realized by using a syringe pump, allowing for very low and constant water injection rates. A series of inflow rates was investigated, namely 0.01, 0.02, 0.03, 0.04, and 0.05 ml/h that represent relevant outflow rates from URLs in granite /KRÖ 19/. These values were also in accordance with the safety limits defined by SKB for the maximum permissible inflow into deposition boreholes of 0.1 l/min /SKB 10/, ensuring the relevance of the experiment for repository conditions.

2.8.2 Modelling Framework

Four modelling teams participated in Task 14a, each applying their respective modelling approaches to simulate the experiment. The modelling code used by GRS was the COMSOL-VIPER interface /KRÖ 23/.

The COMSOL-VIPER interface was originally developed under the project WiGru-9 /NOS 22/ and was further extended within the project SIRUB /KRÖ 26/. The latest development in this context was the implementation of a Neumann boundary condition for one-dimensional applications, enabling direct prescription of inflow rates at the boundary.

This newly implemented boundary condition was tested against the experimental data of Task 14a. The corresponding modelling results from the active modelling teams of the Task Force were presented at the final meeting of the Task Force EBS in Pori 2025, providing a basis for comparison of different modelling approaches.

Fig. 2.24 presents a comparison between the water content profiles obtained from COMSOL-VIPER simulations and the corresponding laboratory measurements after one, two, and three weeks of hydration. The water content is shown as a function of the axial position along the bentonite sample, which begins with 0 at the inflow boundary.

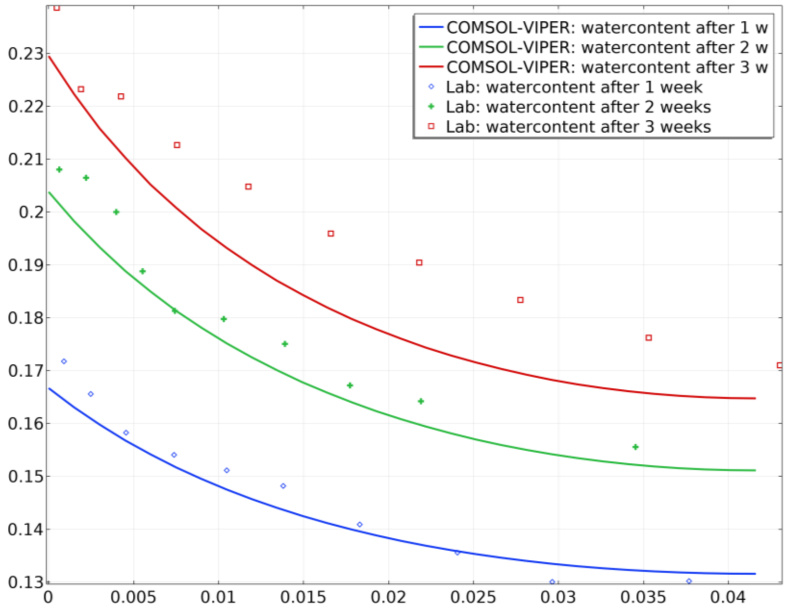

Fig. 2.24 Modelling results (lines) compared to lab data (dotted)

The numerical results exhibit a smooth spatial distribution of water content at all investigated model times. For each time step, the simulated water content is highest near the inflow boundary and decreases monotonically with increasing distance, reflecting the limited water supply conditions imposed at the lower boundary. With increasing hydration time, the overall water content level increases, and the profiles shift upwards while largely preserving their characteristic shape.

The laboratory measurements show the same general trends. The measured data points confirm a local monotonic increase in water content with time while the distribution along the sample length always shows a monotonic decrease. For all three observation times in Fig. 2.24, the highest water contents are observed at the inflow boundary, followed by a gradual decrease towards the upper part of the sample.

A comparison between model results and experimental data indicates good qualitative agreement. The simulated profiles reproduce both the magnitude and the spatial evolution of the measured water contents reasonably well. In particular, the temporal evolution from one to three weeks is consistently captured by the model, demonstrating that the implemented Neumann boundary condition in COMSOL-VIPER is capable of representing the hydration process under constrained inflow conditions.

Some deviations between simulated and measured values are observed, especially at larger distances from the inflow boundary and at later hydration times. The laboratory measurements tend to exhibit slightly higher water contents than the simulated profiles in these regions. These differences may be attributed to uncertainties in the applied effective inflow rate or material heterogeneities.

Overall, the comparison demonstrates that the COMSOL-VIPER model provides a realistic representation of the experimentally observed water content distributions. This supports the suitability of the modelling approach for simulating bentonite hydration under low and controlled inflow conditions.

2.8.3 First comparison of model results

Despite the considerable coordination effort spent at leading Task 14a, a direct comparison of the modelling results from the participating teams was not immediately possible. The primary reason lay in an inconsistency between the applied inflow rates and the resulting accumulated amount of water in the samples. This inconsistency had slipped around the attention of the experimentalists. The inflow rates had therefore been specified in the task description according to the settings of the syringe pump, but the modelling teams found out that these values would lead to a significantly higher water content in the bentonite samples than measured in the laboratory. In practice, significantly lower inflow rates had been assumed for the simulations in order to achieve an agreement with the experimental observations. However, adapted inflow rates had been chosen by each modelling team proactively leading to a certain discrepancy among the numerical models. The results were therefore only qualitatively comparable for the time being.

2.8.4 Analysis of inflow rate uncertainty

The following detailed analysis of the test setup confirmed that the uncertainty of the imposed inflow rates originated from the syringe pump that was used to provide the very low water supply rates. The manufacturer had not provided accuracy specifications for the extremely low flow rates applied in the experiment. Accuracy data were given only for flow rates that were at least one order of magnitude higher than those used in Task 14a. The indicated possible error lay in the range of less than a few percent which had made the experimentalists think to be safe.

To address this issue, additional tests were conducted to evaluate the actual performance of the syringe pump under experiment conditions. The experimental procedure for the pump testing was designed to minimize systematic errors, particularly those arising from evaporation.

In these tests, a syringe filled with water was installed in the syringe pump and connected to a tube. The outflowing water was collected in a beaker. For each target flow rate (0.01, 0.03, and 0.05 ml/h), the pump was operated over a defined period. At regular intervals, the pump was stopped, the syringe was removed and weighed using a precision balance and then reinstalled before restarting the pump. This intermittent weighing procedure was specifically introduced to minimize evaporation effects and improve measurement accuracy. Fig. 2.25, Fig. 2.26, and Fig. 2.27 show the measured flow rates as a function of time for target flow rates of 0.01 ml/h, 0.03 ml/h, and 0.05 ml/h, respectively. In each plot, the red horizontal line indicates the resulting mean flow rate.

For the lowest target flow rate of 0.01 ml/h, the measured values exhibit pronounced temporal variability, as shown in Fig. 2.24. The flow rates fluctuate over a wide range, with individual measurements being systematically lower than the nominal value. Measured flow rates range approximately between 0.0025 ml/h and 0.0095 ml/h with a mean flow of 0.006438 ml/h. No convergence towards the nominal value can be observed over the testing time of 70 days, indicating a rather unstable pump performance at this extremely low flow rate.

At the intermediate target flow rate of 0.03 ml/h, the variability is reduced but still clearly present, see Fig. 2.26. The measured flow rates cluster more closely around the nominal value, with deviations on the order of ±0.002 ml/h or ±6.67 %. The average flow rate of 0.0274 ml/h is much closer to the target value and thereby differs just by 8.7 %. But the individual measurements lie again systematically below the nominal setting.

For the highest tested flow rate of 0.05 ml/h, the measured values show the smallest relative scatter, as shown in Fig. 2.27. The flow rates vary within a comparatively narrow range, approximately between 0.046 ml/h and 0.052 ml/h. Although deviations from the nominal value are still detectable, the relative uncertainty is substantially lower than for the lower flow rate settings as the measured mean flow rate amounts to 0.0487 ml/h corresponding to a difference of 2.6 %. A slight tendency towards increasing measured flow rates with time can be observed, but the limited number of data points does not allow for a conclusive assessment of long-term trends.

Overall, the pump performance measurements clearly demonstrate that the reliability of the syringe pump at the lower end of nominal flow rates strongly decreases with decreasing flow rate settings. In particular, for flow rates on the order of 0.01 ml/h, the observed variability is comparable to the magnitude of the flow rate itself. These findings confirm that the nominal pump settings cannot be considered a sufficiently accurate representation of the actual inflow conditions for the experiment, especially in the low-flow regime relevant for Task 14a.

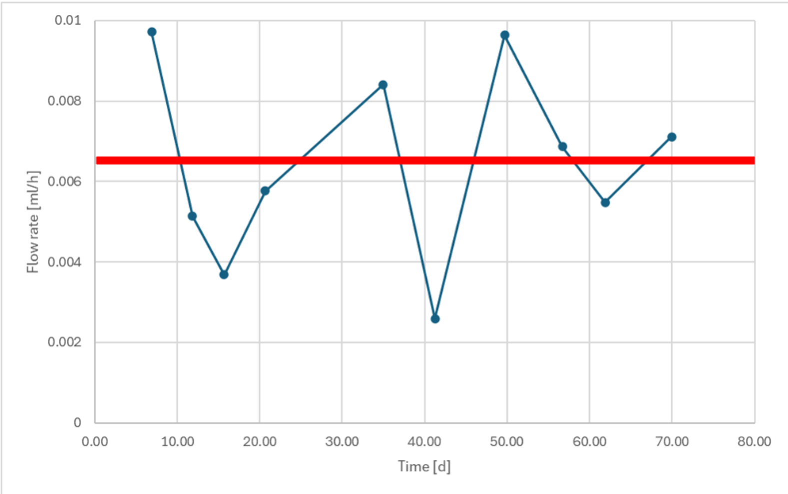

Fig. 2.25 Pump outflow at set 0,01ml/h; red line: mean value

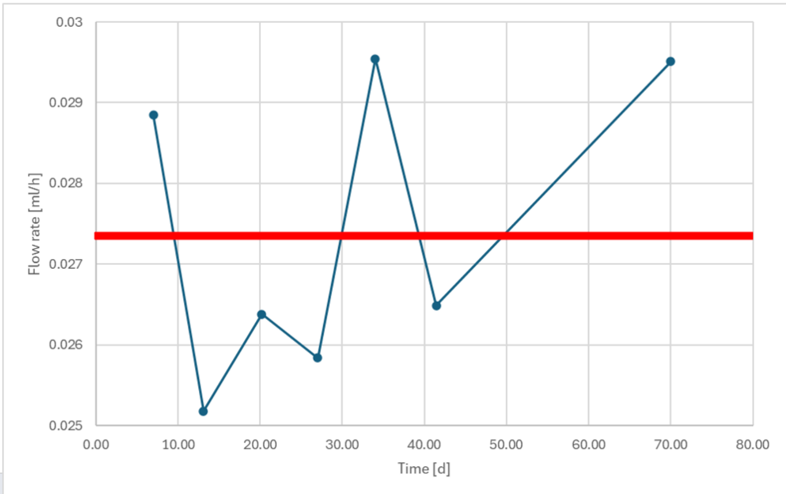

Fig. 2.26 Pump outflow at set 0,03ml/h; red line: mean value

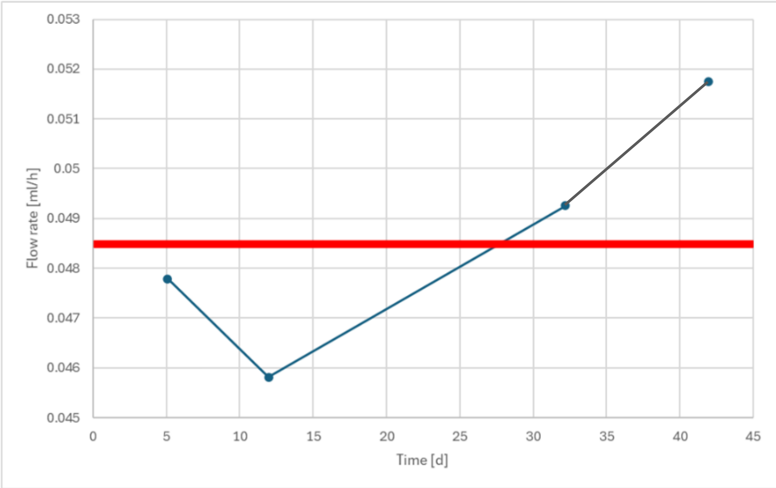

Fig. 2.27 Pump outflow at set 0,05ml/h; red line: mean value

2.8.5 Adopting effective inflow rates

Given the identified limitations of the pump-based flow rate control, it was concluded that the gravimetric water content measurements provided a more reliable basis for quantifying the actual water uptake of the sample. These measurements are inherently less prone to systematic errors compared to the errors at the extremely low flow rates imposed by the syringe pump.

Consequently, it was decided during the final Task Force EBS meeting to redefine the inflow rates based on the new experimental observations. Specifically, effective inflow rates were calculated by dividing the total amount of water absorbed by the sample by the corresponding measurement duration.

This approach provides an integrated measure of the inflow that is consistent with the observed state of the system and independent of the uncertainties in the pump operation.

2.8.6 Final Approach for Model Comparison

In order to ensure a consistent and meaningful comparison between the modelling results, all participating teams agreed to use the recalculated, measurement-based inflow rates for new simulations, as this could be realized with little effort by every modelling team. It is intended to have a joint publication about the resulting final comparison, as soon as all modelling teams have delivered their results.

2.9 CatchNet

The experimental investigations on ice formation in 3D-printed fracture replicas were continued. The objective was to qualitatively observe freezing processes and their impact on the hydraulic conductivity of a fracture under controlled thermal and mechanical conditions.

All experiments were conducted at a constant temperature of −5 °C inside a Weiss climate chamber that provides a temperature stability of ±0.1 °C. Prior to each experiment, the complete experimental setup was tempered for at least 48 hours to ensure a homogeneous and stable temperature distribution throughout the system before commencing observation of the freezing process.

The fracture replica was mechanically confined during the experiments as a relative movement of the two fracture halves widening the fracture had been observed in earlier tests. This effect was believed to be caused by the volumetric expansion of water during freezing. Accordingly, a mechanical constraint was applied to ensure that the hydraulic effects were predominantly related to phase change processes within the fracture's void space. The replica represents a single fracture with a mean aperture of approximately 400 µm.

To visualize flow and freezing processes, a 0.05 % methylene blue solution was used as a tracer. This tracer does not significantly alter the freezing point of water and is commonly used in permafrost-related studies due to its distinct different optical properties in liquid and frozen states. In the recorded images, the tracer appears dark blue in the liquid phase, while a transition towards a clear translucency indicates freezing.

The test results show that ice formation within the fracture occurs rapidly after exposure to freezing conditions but initially remains incomplete. During the early phase of the experiment, a partial freezing within the fracture is observed. The fracture surfaces appear to be covered by a thin ice film, while interconnected liquid pathways remain present within the fracture aperture. During this stage, tracer transport through the fracture is still possible, indicating that water flow is reduced but not entirely suppressed.

Fig. 2.28 shows a processed image sequence illustrating the rapid formation of an ice film within the fracture replica. In the processed images, dark regions correspond to the liquid phase of the tracer solution, while bright regions indicate solidified, frozen areas. This color contrast enables a clear identification of the spatial progression of ice formation.

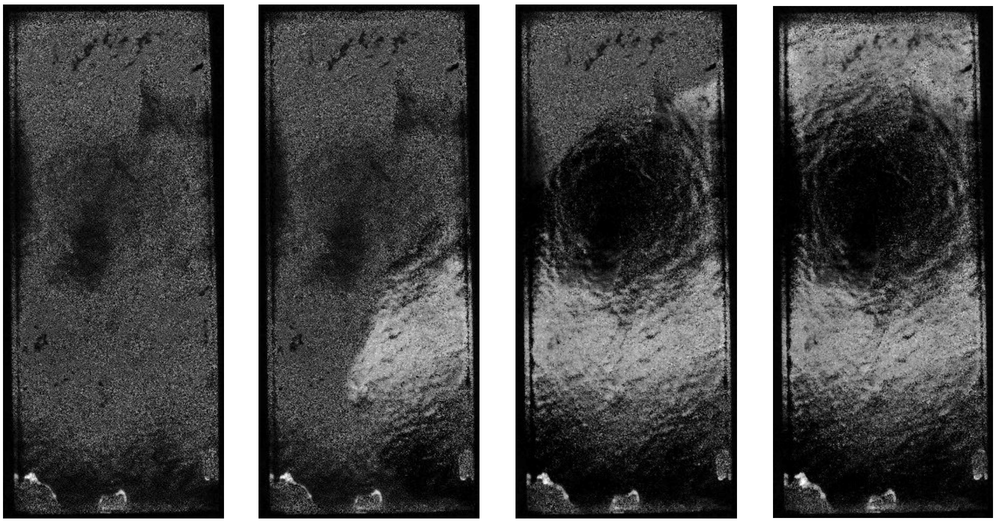

Fig. 2.28 Processed images showing partial freezing in a fracture replica, time from first to last image 4s, bright colour indicates ice

The image sequence captures a short freezing event with a total duration of approximately 4 s from the first to the last frame. Within this time interval, a rapid transition from predominantly liquid conditions to partial ice coverage can be observed. The images indicate that ice formation initiates locally and spreads quickly along the fracture surfaces, resulting in the formation of a continuous ice film.

Despite the rapid development of ice coverage observed in the images, no significant increase in back pressure in the inflow tube was registered during this event. This observation is consistent with the earlier visual findings, suggesting that the initial formation of thin ice films does not immediately lead to a complete hydraulic blockage of the fracture. Instead, it indicates the presence of remaining liquid pathways that allow continued flow during the early stages of freezing.

The circular dark region visible in the middle of the images is attributed to lighting effects and therefore not interpreted as a physical feature of the fracture or indicator of unfrozen zones. These artefacts are consistent visible across multiple frames and remain spatially fixed, supporting their classification as optical effects rather than transient flow or phase-change phenomena.

Following the formation of the initial ice film, a subsequent freezing process was directly observed based on tracer color change. Fig. 2.29 presents cropped sections of images capturing this phenomenon in greater detail. In the images, dark regions represent the liquid tracer phase, while bright regions indicate crystallized tracer.

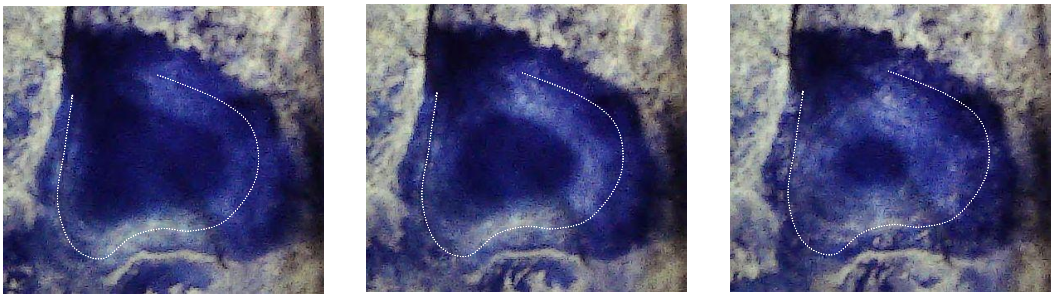

Fig. 2.29 Observed circular freezing front; blue colour shows tracer in liquid state, clear/gray colour indicates cristallized tracer; white dotted line for reference

The image sequence documents a freezing event with a total duration of approximately 1 min 56 s from the first to the last frame. At the beginning of the sequence, the region of interest is predominantly in the liquid state. During the course of the event, a distinct bright ring becomes visible, indicating the formation of solid phase material within the liquid-filled fracture.

This bright ring expands into the dark liquid phase, with freezing progressing mainly inwardly, leading to a gradual reduction of the liquid region enclosed by the ring. The freezing process appears spatially coherent and well-defined, rather than diffuse, highlighting the structured nature of the phase transition within the fracture.

Throughout the observed event, no abrupt changes in the overall image intensity or structure are detected that would indicate mechanical deformation of the fracture. Instead, the evolution is dominated by the gradual replacement of liquid-phase regions by solid-phase material. The comparatively long duration of the second freezing event compared to the rapid ice film formation observed earlier indicates that different freezing mechanisms or controlling processes may be involved.

The observed phenomena allow for several conclusions. Freezing within the fracture does apparently not occur uniformly in space or time. Instead, it proceeds through distinct, localized fronts that propagate through the remaining liquid phase after initial ice formation at the fracture surfaces.

Ice formation within the fracture proceeds apparently through multiple, temporally distinct stages. An initial, very rapid phase is characterized by the formation of thin ice films along the fracture surfaces, occurring on a timescale of only a few seconds. This stage is followed by a slower freezing process within the remaining liquid phase, which evolves over several minutes and is marked by the propagation of well-defined solidification fronts.

During both stages, hydraulic connectivity may persist temporarily, as evidenced by continued tracer transport and the absence of a significant increase in backpressure during the first phase of freezing.

The experimental findings were presented and discussed at the CatchNet meeting 2025, which was held at the EGU in Vienna. The combined visual observations provide robust qualitative insight into the dynamics of fracture freezing under constant subzero temperature conditions. In particular, the identification of transitional regimes in which ice formation and hydraulic transport coexist highlights the complexity of thermo-hydraulic processes in the confined space of fractures. These results contribute to an improved conceptual understanding of freezing-induced permeability evolution and may serve as a valuable qualitative basis for future modelling efforts.

2.10 DECOVALEX

The DECOVALEX-2027 PA Task focuses on the systematic comparison of models and methodologies used for post-closure performance assessment (PA) of deep geological repositories for radioactive waste. Its overarching objectives are to strengthen confidence in PA models, methods, and software, and to foster further research and development in PA methodologies. To achieve these objectives, the task advances PA modelling capabilities by explicitly investigating how modelling choices influence calculated repository performance and by evaluating the relative importance of uncertainties arising from model choices in comparison to other sources of uncertainty.

Within the PA Task, these objectives are pursued through two parallel host-rock–specific activities, namely the PA Salt Task and the PA Crystalline Task, which address performance assessment for repositories in salt and crystalline formations, respectively.

Within the PA Salt Task, these objectives are addressed for disposal concepts in salt formations through the development, application, and comparison of integrated PA models for a reference scenario in domal salt.

The task follows a staged, transparent modelling strategy that enables a systematic evaluation of process coupling and its influence on performance metrics relevant to repository safety. The task is a direct follow-up to DECOVALEX-2023 Task F2, in which participating teams developed and compared deterministic PA models for a generic salt repository using a stepwise approach. That work demonstrated the dominant role of salt compaction and diffusive transport for the scenarios considered, while also highlighting limitations related to process representation, coupling strategies, and the lack of systematic uncertainty treatment /LAF 23/.

In the present phase of DECOVALEX-2027, the generic PA framework developed previously has been extended and refined to explicitly address these limitations. Participating teams began by implementing a set of benchmark cases that separately address diffusion-dominated transport processes and salt creep behavior. These benchmark cases provided a common basis for model comparison and code verification across the participating teams. In addition, uncertainty and sensitivity analyses will be conducted for the benchmark cases, representing an important first step toward a more comprehensive and systematic treatment of uncertainty within integrated PA models for repositories in salt formations.

2.10.1 Task Objectives and Structure

The task outline structure for the salt (S) subtask (Task PA) is as follows:

- Step 0S: Develop numerical models from the DECOVALEX-2023 Task Specification. Returning teams update/improve DECOVALEX -2023 model (full-scale or whole repository model) as needed.
- Step 1S: Salt Reference Case Process Model Comparison via benchmark cases for diffusion and salt creep (benchmark models). Compare performance measures or other outputs from test cases or subsystem process models.
- Step 2S: Heat generation and gas generation associated with steel corrosion (full-scale or whole repository model). To account for additional physics, teams may wish to utilize sub-models, or other methods, to investigate gas generation at the waste package scale and implement those results to the repository scale.

- Step 3S: Uncertainty quantification and Sensitivity Analysis with a primary focus on creep closure models and diffusive transport (benchmark models).
- Step 4S: Uncertainty quantification and Sensitivity Analysis of the reference case. Here, generating samples for creep closure and diffusion models, propagate the “model form” uncertainty through the reference case simulation, and perform analysis (full-scale or whole repository model, from Step 0 or Step 2) is the first step. Definition of constitutive model types (e.g. different creep closure models) will be specified and parameterized for SA. Perform SA for various model form choices. In the second step, the closure model and diffusion model uncertainty with parameter uncertainty are combined, and a combined analysis is performed. Combine model form uncertainty with parameter uncertainty, perform combined sensitivity analysis (full-scale or whole repository model, from Step 0 or Step 2).

2.10.2 Benchmark description

To compare performance measures and other outputs in a first step, simple test cases or subsystem process models are established. This can be used to understand differences in model implementation and how modelling choices affect calculated values. As the previous DECOVALEX phase showed that salt compaction and radionuclide diffusion are the key physical processes to consider, /LAF 23/ there was a Diffusion and Creep Benchmark set up.

For the **Diffusion Benchmark** the assumptions made include:

- Purely diffusive transport of an ideal tracer in an isotropic porous media.
- A semi-infinite domain, $r > 0$, in 1D, 2D (radial) or 3D (spherical) coordinates.
- The tracer is introduced at a point source.
- The media is saturated with single-phase resident fluid, which is assumed to be brine.
- The porosity of the domain is a function of radius.
- Diffusive transport is controlled by the effective molecular diffusion coefficient. Diffusion is a function of porosity, and thus a function of radius through porosity in this model.

- The mass balance equation in arbitrary dimension m = 0, 1, or 2 is given by /BAT 06/.

Subsequently, teams produce six Benchmarks. As shown in Tab. 2.3 and Tab. 2.4, Benchmarks 1-3 are diffusion in a homogeneous domain with a constant source for 1D, 2D and 3D cases with a constant porosity. Benchmarks 4-6 are diffusion through the heterogeneous domain with a constant source for 1D, 2D and 3D cases. Porosity is decreasing as a power law with radius from the source. Tortuosity is modeled as function of porosity. The analytical solutions are shown in Fig. 2.30 to Fig. 2.33.

Tab. 2.3 Diffusion benchmark models with a constant source

Name	Dimensionality	Porosity	Diffusivity	Comparison radius (m)	Comparison time (yr)
BM 1	1D	ϕ_0	D_0	r = 1.0	t = 100.
BM 2	2D	ϕ_0	D_0	r = 1.0	t = 100.
BM 3	3D	ϕ_0	D_0	r = 1.0	t = 100.
BM 4	1D	$\phi_0(r/r_w)^{-\eta}$	$AD_0(\phi)^\gamma$	r = 0.2	t = 100.
BM 5	2D	$\phi_0(r/r_w)^{-\eta}$	$AD_0(\phi)^\gamma$	r = 0.2	t = 100.
BM 6	3D	$\phi_0(r/r_w)^{-\eta}$	$AD_0(\phi)^\gamma$	r = 0.2	t = 100.

Tab. 2.4 Parameters for the diffusion benchmark models

Parameter	Value
$r_w[m]$	0.1
$\phi_0[-]$	0.1
$\eta[-]$	BM 1-3: 0.0 BM 4-6: 4.5
$\gamma[-]$	BM 1-3: 0.0 BM 4-6: 0.5
$A[-]$	1; 0
$D_0[m^2/s]$	1×10^{-9}

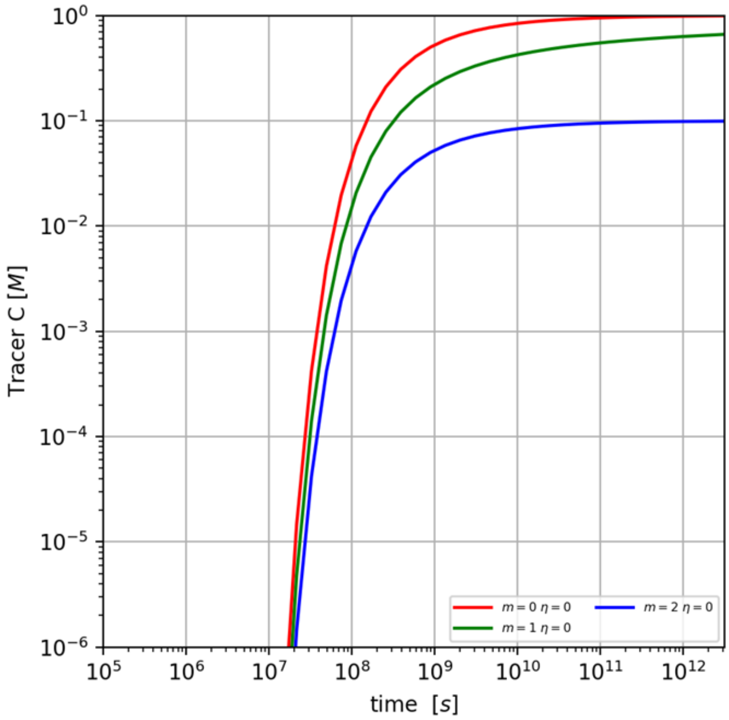

Fig. 2.30 Tracer profiles as a function of time at r = 1.0 m for homogeneous diffusion constant source benchmark cases BM 1-3. Red is the 1D solution (BM 1), green is the 2D-radial solution (BM 2) and blue is the 3D-spherical solution (BM 3)

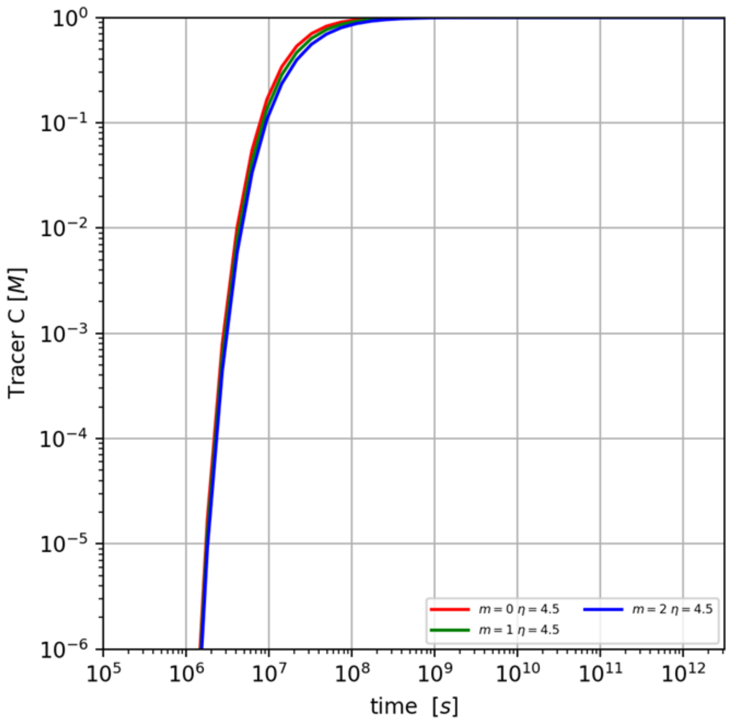

Fig. 2.31 Tracer profiles as a function of time at r = 0.2 m for decreasing porosity and diffusivity diffusion constant source benchmark cases BM 4-6. Red is the 1D solution (BM 4), green is the 2D-radial solution (BM 5) and blue is the 3D-spherical solution (BM 6)

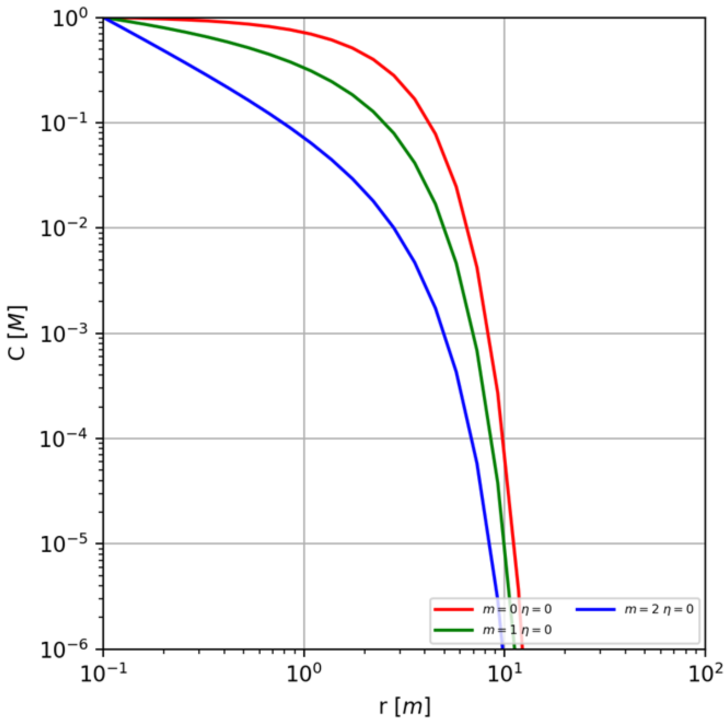

Fig. 2.32 Tracer at time t = 100 years as a function of radius for homogeneous diffusion benchmark cases with constant source BM 1-3. Red is the 1D solution (BM 1), green is the 2D-radial solution (BM 2) and blue is the 3D-spherical solution (BM 3)

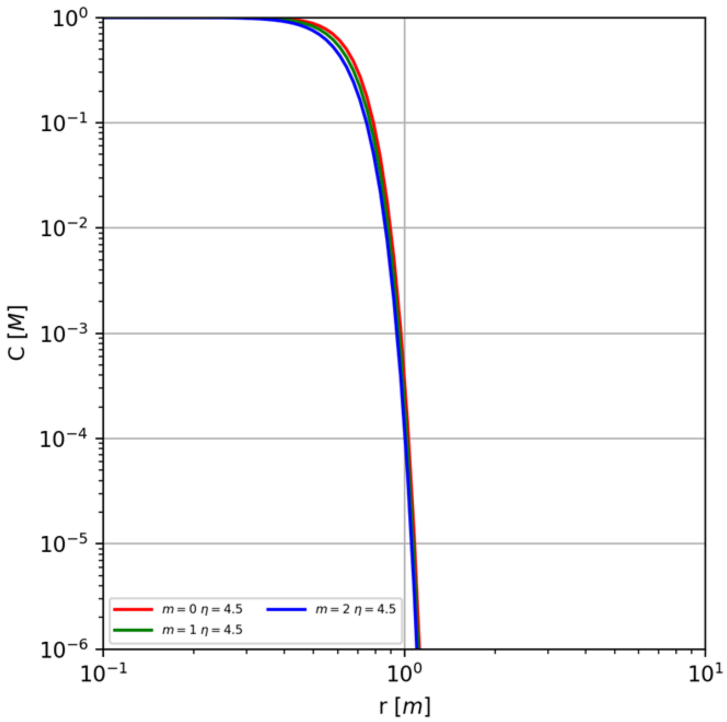

Fig. 2.33 Tracer at time t = 100 years as a function of radius for decreasing porosity and diffusivity diffusion benchmark cases with constant source BM 4-6. Red is the 1D solution (BM 4), green is the 2D-radial solution (BM 5) and blue is the 3D-spherical solution (BM 6)

For the **Creep Closure Benchmark** some simplifying assumptions are made. Firstly, the volume is considered constant, subsequently it is also assumed that the system is isothermal.

- A one-dimensional flow of a slightly compressible single-phase fluid is calculated.
- Porosity is a function of space and time only through the gas pressure. This is equal to the assumption of a constant volume as mentioned above.
- Permeability and viscosity are constant in space and time. his represents a second simplification from the reference case model, as in general permeability decreases exponentially with porosity.
- No sources/sinks.

This benchmark case is to simulate porosity and pressure in a dry, air-filled tank model. Teams compare pressure and porosity as a function of time for (0.01,100) years for either a single grid-cell model and/or the average pressure and porosity for a multi-cell model. The analytical solution is given in Fig. 2.34.

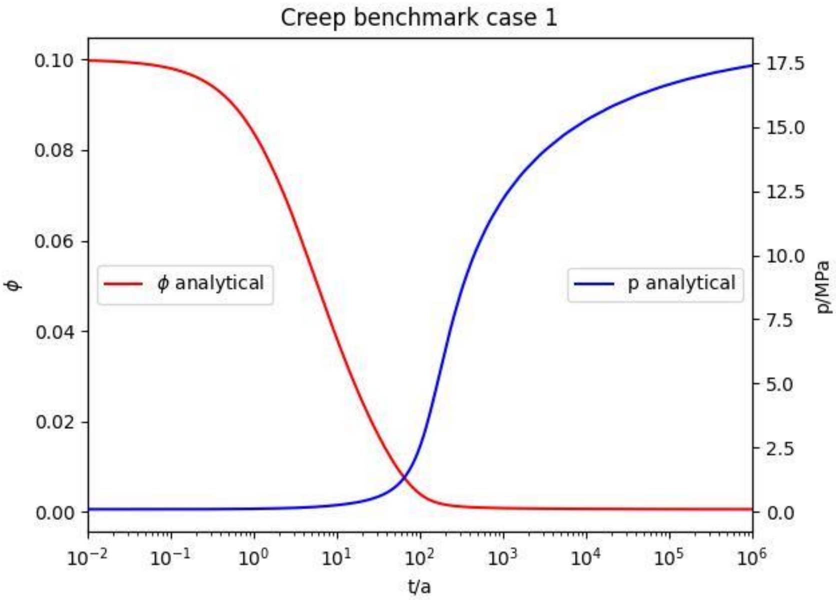

Fig. 2.34 Numerically integrated porosity and pressure for an air-saturated tank using the creep closure parameters in Tab. 2.4

2.10.3 Modelling approach

The participating teams include the Federal Office for the Safety of Nuclear Waste Management (BASE), which serves as the German government's central authority responsible for the safe management of the legacy of nuclear energy. The consortium also involves the Central Organization for Radioactive Waste (COVRA), the sole organization in the Netherlands authorized to collect, process, and store all Dutch radioactive waste. In addition, Quintessa, a UK-based scientific and technical consultancy specializing in radioactive waste management and safety assessment, and GRS (Gesellschaft für Anlagen- und Reaktorsicherheit), a leading German technical safety organization with extensive expertise in nuclear safety and radioactive waste disposal, are participating.

Across the benchmarks, the participating teams employed different software tools, and individual teams may have used more than one tool. Tab. 2.5 provides an overview of the applied software. BASE for example used TOUGH-2 for the creep benchmark as they had already implemented dedicated approach within this framework to represent salt creep processes. Besides, their aim is to use PFLOTRAN for the diffusion benchmark and the subsequent full-scale model in the years ahead. GRS used Claypos for the diffusion benchmark as it is particularly suited to the analysis of diffusion-controlled processes, and NATREND in order to further test and validate the code within the scope of the study. For the creep benchmark and future full-scale model, LOPOS is chosen. COVRA employed COMSOL, a flexible finite-element platform for coupled process modelling, whereas Quintessa used QPAC, its in-house multi-physics performance assessment code, enabling fully coupled simulations.

Tab. 2.5 Teams' Software and Features used in the Benchmarks

Team	BASE		COVRA	GRS			Quintessa
Software	PFLOTRAN	TOUGH-2	COMSOL	CLAYPOS	LOPOS	NATREND	QPAC
Benchmark Case	Diffusion	Creep	Diffusion Creep	Diffusion	Creep	Creep	Diffusion Creep
Dimensionality	3D	3D	1D/2D	1D	1D	3D	3D
Solution Method	Finite Volume	Finite Volume	Finite Element	Finite Volume	Finite Volume	Finite Volume	Finite Volume / Mixed Element
Conceputal Model Type	Continuous	Continuous	Continuous	Compartment			Continuous
Phases	Multi-Phase	Multi-Phase	Multi-Phase	1-Phase	1-Phase	Multi-Phase	Multi-Phase

2.10.4 Results

In this chapter, representative example results are presented to document the progress achieved so far. The results are shown in their current form, which does not yet allow for a fully consistent visual comparison across all cases. In addition, results and explanatory input from all partners are not yet available. The figures should therefore be understood as indicative rather than exhaustive.

2.10.4.1 Diffusion Benchmark

Fig. 2.35 shows the evolution of tracer concentration as a function of time. Three curves are displayed: a red line representing the one-dimensional homogenous Benchmark case 1 (BM 1), a green line representing the radial homogenous Benchmark (BM 2), and a blue line representing the spherical homogenous Benchmark (BM 3). Darker shades represent the analytical solution as also shown in Fig. 2.30, lighter colors represent the CLAYPOS results. All curves exhibit a monotonic increase in tracer concentration with time and approach a steady-state plateau at late times and there is very good agreement between the CLAYPOS and analytical solutions. Fig. 2.36 shows the preliminary results for Benchmark cases BM 1 and BM 2 with the newly developed module NATREND.

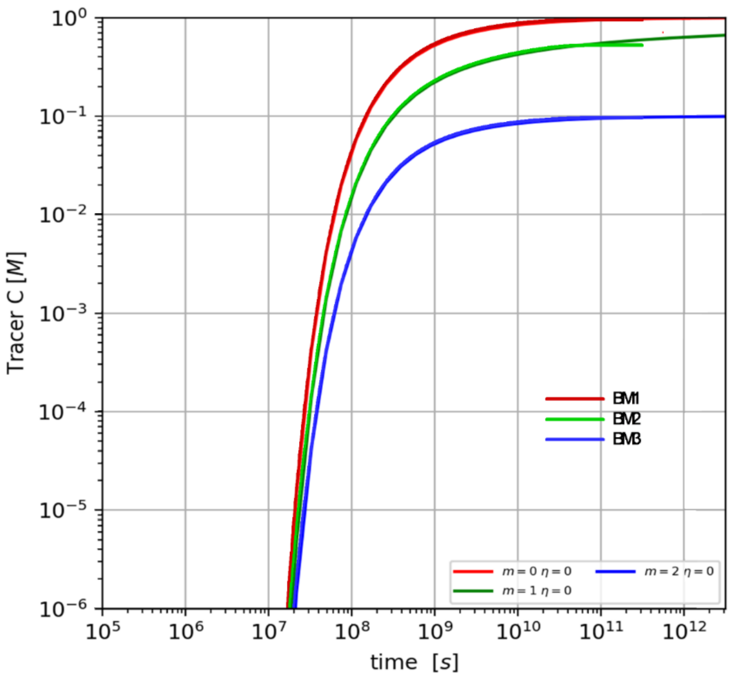

Fig. 2.35 Homogenous Diffusion Benchmarks 1-3 results reproduced by CLAYPOS with tracer profiles as a function of time at r = 1.0 m

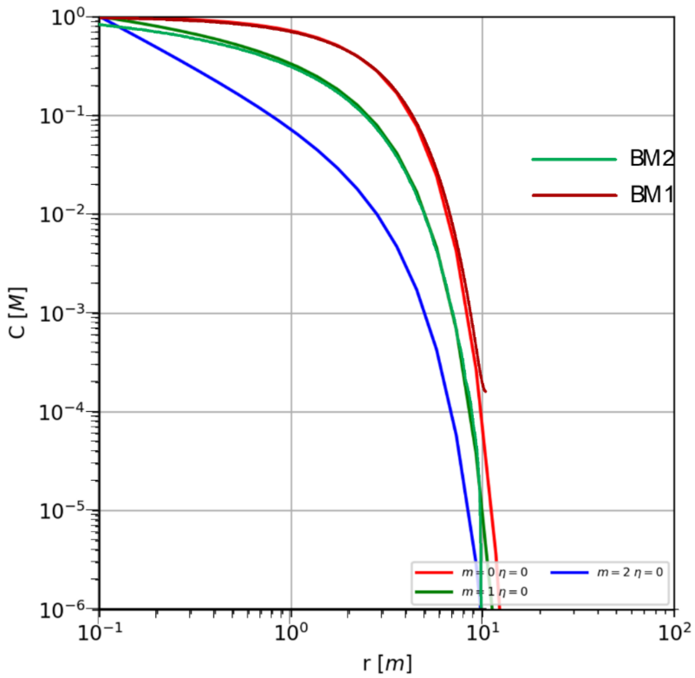

Fig. 2.36 Homogenous Diffusion Benchmark results from GRS reproduced by NATREND with tracer profiles as a function of time at r = 1.0 m

The results for the heterogenous one-dimensional, radial and spherical Benchmark cases (BM 4-6) calculated with PFLOTRAN (in dashed lines) plotted against the analytical solutions (in solid lines) are shown in Fig. 2.37. Here, the radial distribution of the tracer concentration at 100 years is shown.

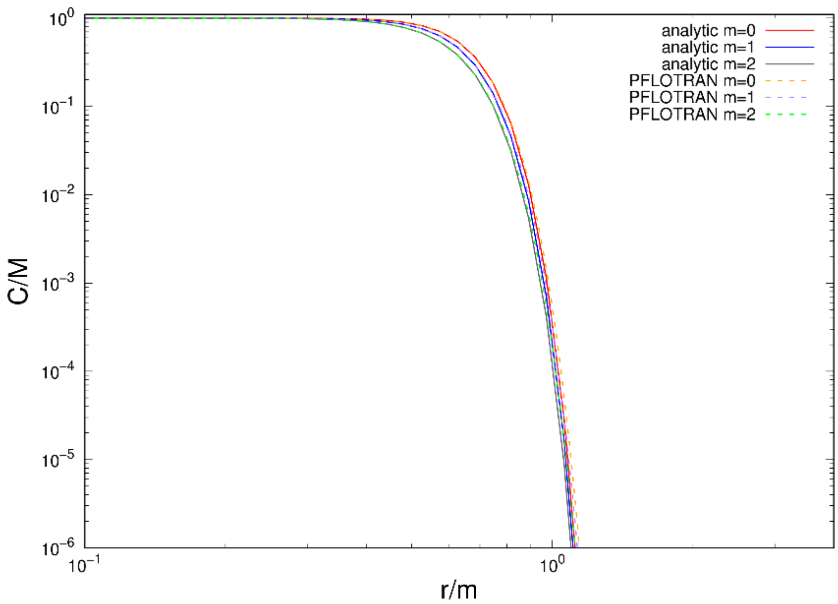

Fig. 2.37 Heterogenous Diffusion Benchmarks BM 4-6 results reproduced by PFLOTRAN with tracer profiles at time t = 100 years as a function of radius

2.10.4.2 Creep Benchmark

Fig. 2.38 shows the analytical solution with the change of porosity in red and the gas pressure in blue over time. The evolution of the porosity calculated by TOUGH2-GRS in dashed black lines and the evolution of gas pressure as dashed yellow line. It should be noted, as in TOUGH2-GRS f_p neglects the dependence on z and is slightly modified the analytical solution was tweaked accordingly. Subsequently, TOUGH2-GRS resembles the analytical solution very well as shown in Fig. 2.38.

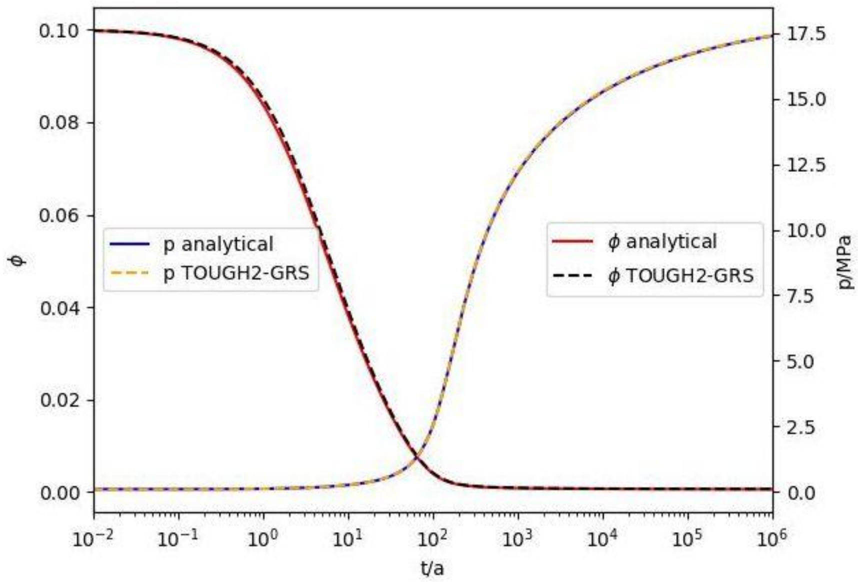

Fig. 2.38 Creep Benchmark results reproduced by TOUGH2-GRS using the creep closure parameters in Table 2.

Quintessa adjusted the constant volume assumption of the analytical solution and thus also reached a perfect agreement with the analytical solution (Fig. 2.39).

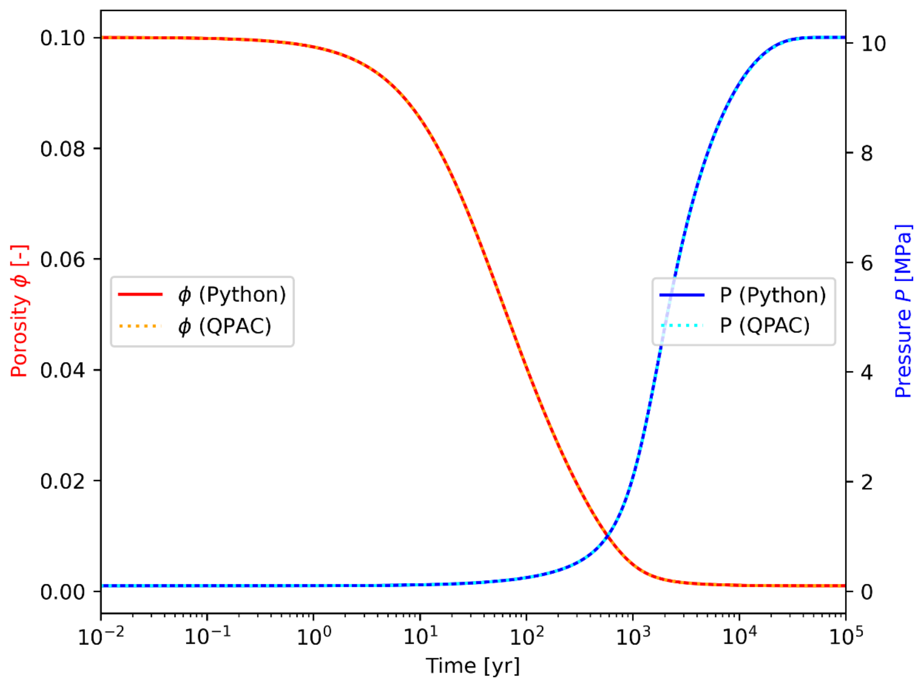

Fig. 2.39 Creep Benchmark results reproduced by QPAC using the creep closure parameters in Tab. 2.4

Fig. 2.40 shows the results from LOPOS. LOPOS is not designed to calculate compression of initial air in pore space; therefore, the benchmark case cannot be fully pictured as the pressure remains constant at 0.1 MPa. Subsequently, the convergence support due to pressure increase is missing and no pressure dependent increase of moisture-enhanced creeping can be observed.

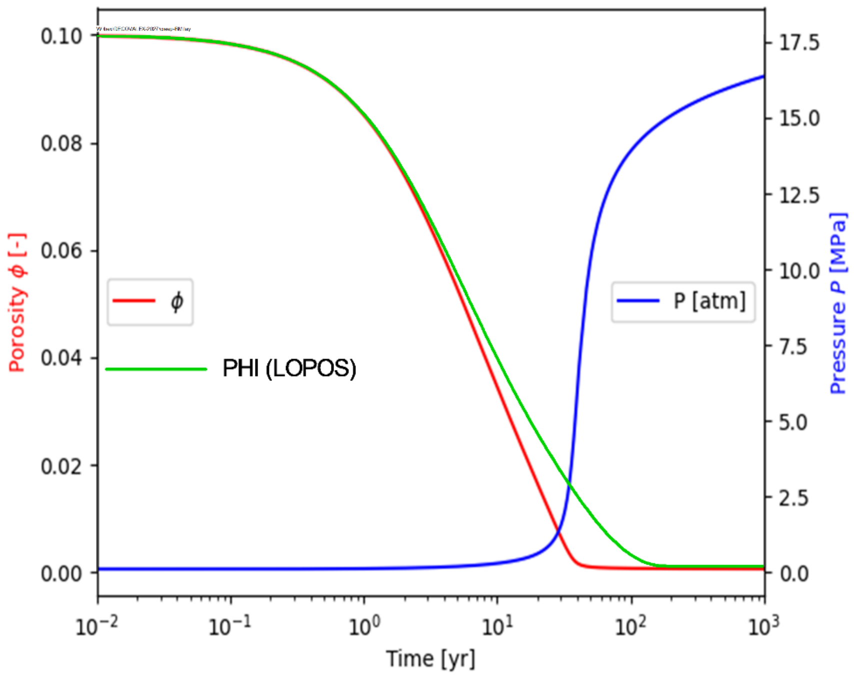

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Fig. 2.40 Creep Benchmark results reproduced by LOPOS using the creep closure parameters in Tab. 2.4

In order to further approach the analytical solution, the following aspects were modified:

- In LOPOS, the aspect of pre-history of convergence is set to 1 instead of 0.2 as given in the table with the input parameter as this parameter is not considered in the script for the analytical solution.
- The simplified assumption of constant volume in the script is removed.
- Moisture creep in LOPOS is set to 4 and the pressure limit set to 0.

As a result, shown in Fig. 2.41, the two curves converge very closely. The remaining minor deviation can be attributed to the fact that increasing air pressure is not taken into account in LOPOS.

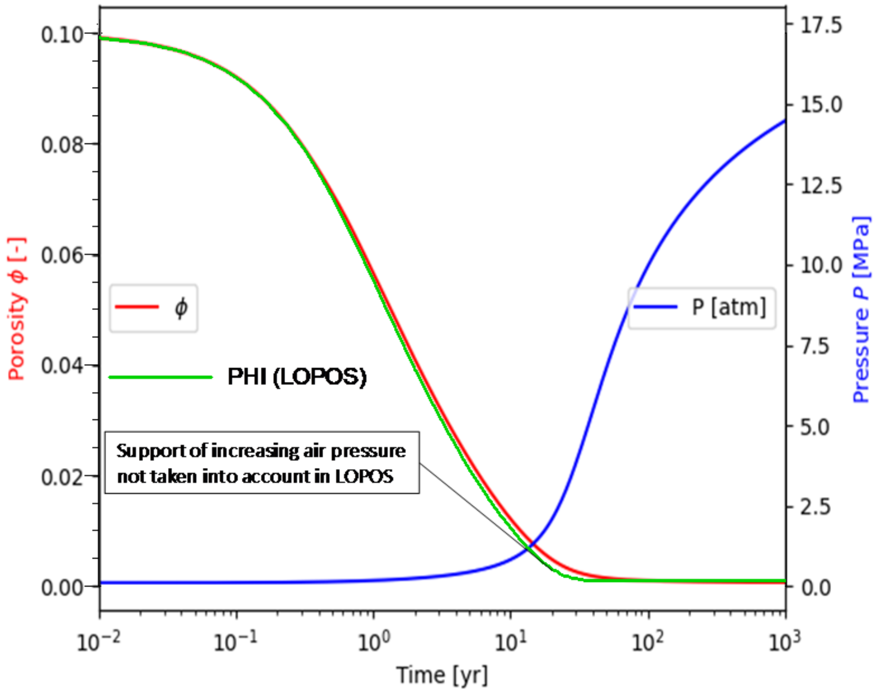

Fig. 2.41 Creep Benchmark results from GRS reproduced by LOPOS

2.10.5 Summary and Outlook

Very good agreement was observed among the participating teams with respect to the analytical solution of the diffusion benchmark. In the creep benchmark, only minor deviations were found. These deviations can be explained by differences in the underlying calculation approaches, and an adjustment of the analytical solution successfully resolves this issue. In the next steps of the study, uncertainty and sensitivity analyses will be carried out for the benchmarks considered. In addition, uncertainty and sensitivity analyses will be performed for an extended reference case derived from DECOVALEX-2023.

3 Summary and conclusions

The methodology for safety assessment of geological repositories, known as the "Safety Case", is well-established within an international framework; it has been applied for over twenty years and is continuously refined, particularly within committees of the Nuclear Energy Agency (NEA) and the International Atomic Energy Agency (IAEA). While this general approach to safety assessment must align with national regulatory frameworks, it should also be internationally accepted; consequently, it requires continuous adaptation to international developments as well as to new insights emerging from research, science, and technology. This project has contributed to deepening the understanding of the Safety Case concept, evaluating new findings from international research for use in national safety demonstrations, and further developing the methodology for long-term safety assessments in accordance with the state of the art.

A key objective of the project is active participation in international committees and working groups to monitor new developments in other countries and at the international level, and to contribute to the development of strategies, methods, and tools for demonstrating the safety of deep geological repositories. Active participation has taken place, on the one hand, within the working groups of the OECD-NEA, specifically the Integration Group for the Safety Case (IGSC), the Working Party on Information, Data and Knowledge Management (WP-IDKM), and corresponding expert groups such as the Salt Club, the Clay Club, and the Crystalline Club. On the other hand, participation in international working groups and projects, including the Joint Sensitivity Analysis Exercise (JOSA), the Task Force on Engineered Barriers (EBS), CatchNet, and DECOVALEX-2027, has played a significant role.

A key focus of the IGSC's work during the duration of this project was the successful organization, evaluation, and publication of the proceedings of the 2024 Safety Case Symposium in Budapest. Inspired by this symposium, the Next Generation Network (NGN) has now become established within the IGSC; since October 2025, it has formally functioned as an *ad hoc* group of the IGSC. The overarching objectives of the NGN are to foster professional development, integrate new voices into the community, promote structured knowledge transfer, and build diverse professional networks. Finally, work continued on the IGSC-GeneSiS project, which compiles experiences gained from the preparation of safety cases – ranging from generic phases to site-specific phases – with the aim of serving as guidance and support for countries currently in the early stages of their deep geological repository programs. Drafts of the final reports for this project are now available and will undergo review by the NEA's committees and working groups in 2026 prior to publication.

Within the NEA's Salt Club, GRS was primarily involved in the work of the NEA Salt Club Working Group on "The role of scenarios in the modelling strategy for the safety assessment for deep geological repositories." This working group is currently examining methods for mapping scenarios onto numerical models (and vice versa). While the aggregate set of selected scenarios covers the uncertainties regarding the future evolution of a repository system, the precise manner in which the scenario approach is linked to the overall modeling strategy remains unclear. Currently, no recommendations exist regarding how to address scenario-related uncertainties within the framework of a modeling strategy designed to cover timeframes of up to one million years. This Salt Club initiative is being conducted in the context of an analysis of national programs for deep geological repositories situated in salt formations. As a starting point, a questionnaire was developed to capture experiences and possibilities regarding the link between scenarios and the modeling strategy.

The NEA Clay Club has made significant progress in understanding clay-rich rocks as host rocks for the geological disposal of radioactive waste. Activities in 2024 focused on a workshop regarding pore-water chemistry and a project investigating pressure anomalies. Studies on pressure anomalies indicate that clay formations typically exhibit underpressure, driven by geological processes such as erosion. New models are improving the interpretation of measurement data and highlighting the importance of long-term monitoring. Overall, the results confirm the suitability of clay formations as safe barriers while simultaneously underscoring the need for detailed, site-specific analyses. The 2025 publication from the CLAYWAT project provides a comprehensive description of new insights into water behavior within nanopores.

The NEA Crystalline Club fosters international exchange aimed at understanding crystalline rocks as host rocks for the deep geological disposal of high-level radioactive waste. During the 2024–2025 period, its work focused on two key topics, namely on chemical conditions relevant to the behavior of a repository in crystalline rock and specifically their impact on the corrosion of disposal canisters, as well as on assessing the feasibility of a "Catalogue of Characteristics" for crystalline rocks. A major outcome was the creation of an extensive literature database (Cryschem) containing over 600 entries, scheduled for publication in 2026. Discussions are currently ongoing regarding whether a "Catalogue of Characteristics", including an analysis of risks, challenges, and a potential roadmap, can be implemented by individual countries.

Radioactive waste originates from a wide variety of sources, encompassing the entire nuclear fuel cycle as well as diverse fields of application in industry, medicine, defense, and research. This waste requires long-term disposal. The timelines for radioactive waste disposal programs – from their inception to the final closure of the repository – typically span many decades. These extended timeframes present complex challenges that extend across multiple generations of technical experts and various stages of technological development. Throughout the course of a disposal program, a vast volume of data and information is generated. Given the challenges associated with managing this critical information, many countries are currently exploring the development of a "Digital Safety Case" – an innovative approach designed to comprehensively track and document processes within the field of radioactive waste disposal. Furthermore, many countries are beginning to select and compile a structured *Set of Essential Records* (SER) from this wealth of data and information. The aim is to ensure that future decision-makers are able to effectively manage the hazards associated with radioactive waste throughout its entire lifecycle. Moreover, there is a growing trend toward collaborative efforts in developing strategies to preserve knowledge regarding radioactive waste repositories over extremely long timeframes. These aspects are being addressed internationally, particularly by the NEA Working Party on "Information, Data and Knowledge Management" (WP-IDKM), and were presented to and discussed with the international community at the 2025 Symposium in Yokohama. A further aspect of current work concerns the extent to which modern technologies such as artificial intelligence can contribute to these topics, for instance, in the selection and compilation of essential records.

GRS continued in participating the JOSA (Joint Sensitivity Analysis Exercise), which is an international collaboration to test and investigate probabilistic sensitivity analysis methods in application to realistic numerical models in the context of radioactive waste disposal. In 2025 the third phase of JOSA was started. As one of the topics addressed in the third phase GRS work focused on investigation of screening methods, particularly on the Morris screening method. This method is based on the effects on the model output caused by small local changes of individual parameters, called elementary effects.

Within Task 14a of the Task Force EBS, led by GRS, the capability of different modelling approaches to reproduce the hydraulic behavior of compacted MX-80 bentonite under limited water supply was systematically investigated. A series of laboratory experiments, performed by GRS within the Project WiGru-7 /NOS 18/, provided a valuable reference dataset for the task. The comparison of numerical simulations with the underlying experimental observations demonstrates that the applied modelling approaches, particularly the COMSOL-VIPER interface, are generally able to capture the key features of bentonite hydration. This confirms also the suitability of the recently implemented Neumann boundary condition in the COMSOL-VIPER interface for representing limited inflow conditions. However, the comparison revealed significant uncertainties related to the experimental boundary conditions, specifically the accuracy of the syringe pump at very low flow rates. Pump performance tests proved that actual flow rates could deviate substantially from the nominal settings. This finding explains the initially observed discrepancies between modelling results and experimental data and highlights the importance of carefully verifying boundary conditions in such experiments. By adopting effective inflow rates derived from the gravimetric measurements, a consistent basis for model comparison was established. This approach allows for a more meaningful comparison of modelling results with the experimental results as well as across the participating teams. A final quantitative comparison is currently being prepared and planned to form the basis of a joint publication.

Complementary experimental work concerning the CatchNet utilizing 3D-printed fracture replicas provided new qualitative insights into freezing processes in fractures. The observations demonstrate that ice formation in a fracture occurs in multiple stages, starting with rapid ice film formation along fracture surfaces, followed by a slower propagation of localized freezing fronts. Importantly, hydraulic connectivity may persist during early freezing stages, indicating a complex interplay between phase change and flow processes. The results highlight the non-uniform and transient character of phase-changes in fractures and emphasize the relevance of resolving the spatially heterogeneous freezing process when assessing permeability evolution in fractures under freezing conditions.

The Joint Sensitivity Analysis Group (JOSA) was established seven years ago. The focus of JOSA's work lies in the application of sensitivity analyses (SA) to selected computational cases, with the overarching goal of developing and providing guidelines for conducting such analyses within the context of safety assessments for geological repositories. The objective of this work is to gain a better understanding of the strengths and weaknesses of various SA methods, to determine the performance capabilities of these methods, and to identify best practices and other insights derived from the benchmark study. Phase 3 of JOSA commenced in 2025. As one of the topics addressed during this third phase, GRS focused its efforts on investigating screening methods—specifically, the Morris screening method. This method examines parameter sensitivity based on the impact that small, localized changes to individual parameters have on the model output. The results of the GRS model calculations for a repository containing low- and intermediate-level radioactive waste suggest that, in such a complex case, large sample sizes, comprising at least 1,000 trajectories, and well-structured Morris samples are required to minimize outliers and irregularities in the resulting Morris sensitivity measures; such anomalies would otherwise significantly hinder the classification of parameters as highly important, less important, or (virtually) unimportant. The LILW case exhibits complex behavior, including quasi-discrete characteristics, that can lead to abrupt shifts in model output values. The Morris method appears to be well-suited for identifying all potentially significant parameters and interactions using a relatively small number of model runs. The Morris method is not suitable for classifying the full range of significance levels for various parameters and interactions, as it was designed as a screening procedure rather than as a quantifying method, such as variance-based sensitivity analysis. Ultimately, a major advantage of the Morris method lies in its ability to reduce the number of parameters for subsequent, in-depth analyses, for instance, by means of variance-based or other methods.

One task of the DECOVALEX project focuses on the systematic comparison of models and methods employed in the long-term safety analysis (PA) of radioactive waste repositories. Within the scope of this comparison, two parallel, host-rock-specific activities are being pursued, namely the "PA Salt Task" and the "PA Crystalline Task", which address, respectively, the safety assessment of repositories situated in salt and crystalline formations. This report reviews the project-supported work concerning repositories in salt formations. In the current phase of the project, the participating modelling teams have commenced the implementation of a series of benchmark cases, each separately addressing diffusion-dominated transport processes and the creep behaviour of salt. The results of the benchmarks obtained to date demonstrate that, with regard to the analytical solution of the diffusion benchmark, a very high degree of agreement has been achieved among the participating teams. Only minor discrepancies were observed in the creep benchmark. These discrepancies can be attributed to differences in the underlying computational approaches; an adjustment of the analytical solution successfully resolves this issue. In the subsequent stages of the study, uncertainty and sensitivity analyses will be conducted for the benchmarks under consideration. Furthermore, uncertainty and sensitivity analyses will be performed for an extended reference case derived from DECOVALEX-2023.

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ISBN 978-3-911727-51-8