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Performance Assessment Methodologies in Application to Guide the Development of the Safety Case

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FULLY PROBABALISTIC SAFETY ASSESSMENT DELIVERABLE (D-N°: D2.2.E.1)

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Foreword

The work presented in this report was developed within the Integrated Project PAMINA: **P**erformance **A**ssessment **M**ethodologies **IN A**pplication to Guide the Development of the Safety Case. This project is part of the Sixth Framework Programme of the European Commission. It brings together 25 organisations from ten European countries and one EC Joint Research Centre in order to improve and harmonise methodologies and tools for demonstrating the safety of deep geological disposal of long-lived radioactive waste for different waste types, repository designs and geological environments. The results will be of interest to national waste management organisations, regulators and lay stakeholders.

The work is organised in four Research and Technology Development Components (RTDCs) and one additional component dealing with knowledge management and dissemination of knowledge:

- In RTDC 1 the aim is to evaluate the state of the art of methodologies and approaches needed for assessing the safety of deep geological disposal, on the basis of comprehensive review of international practice. This work includes the identification of any deficiencies in methods and tools.

- In RTDC 2 the aim is to establish a framework and methodology for the treatment of uncertainty during PA and safety case development. Guidance on, and examples of, good practice will be provided on the communication and treatment of different types of uncertainty, spatial variability, the development of probabilistic safety assessment tools, and techniques for sensitivity and uncertainty analysis.

- In RTDC 3 the aim is to develop methodologies and tools for integrated PA for various geological disposal concepts. This work includes the development of PA scenarios, of the PA approach to gas migration processes, of the PA approach to radionuclide source term modelling, and of safety and performance indicators.

- In RTDC 4 the aim is to conduct several benchmark exercises on specific processes, in which quantitative comparisons are made between approaches that rely on simplifying assumptions and models, and those that rely on complex models that take into account a more complete process conceptualization in space and time.

The work presented in this report was performed in the scope of RTDC 2.

All PAMINA reports can be downloaded from http://www.ip-pamina.eu.

Arbeitsbericht NAB 10-37

PAMINA RTDC-2

Deliverable D2.2.E.1

Fully Probabilistic Safety Assessment

December 2010

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This report was prepared by Johannes Holocher (AF-Colenco) and Jürg Schneider (Nagra). Chapter 5 was written by José Luis Cormenzana (ENRESA) and published as Milestone Report M2.2.E.4. The work described in this report was supported by a working group consisting of (in alphabetical order) Stefan Finsterle (LBNL), Peter Gribi (S+R Consult GmbH, Baden), Georg Kosakowski (PSI), Ulrich Kuhlmann (TK Consult), Paul Marschall (Nagra), Gerhard Mayer, Joachim Poppei, Georg Resele (AF-Colenco), Peter Robinson (Quintessa), Christian Sprecher (Sprecher Consulting GmbH, Wettingen) and Piet Zuidema (Nagra).

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1 Introduction

1.1 Background and objectives

The development of an integrated approach for a fully probabilistic safety assessment (PSA) in the context of the evaluation of long-term safety for deep geological repositories is of strategic interest to the Swiss National Cooperative for the Disposal of Radioactive Waste (Nagra). For that reason, Nagra had started such a project some time before the beginning of the PAMINA project. Discussions with other potential PAMINA project partners prior to the start of PAMINA showed that this topic is of wider interest. Nagra then suggested sharing the experience gained during this project with the PAMINA participants, which eventually led to the inclusion of Task 2.2.E in PAMINA.

The main objective of Task 2.2.E was to develop and test an integrated approach for a fully probabilistic safety assessment (PSA) and the necessary tools. Additional objectives included the realisation of a set of corresponding independent complementary calculations using existing software tools, and a review of the regulatory situation regarding probabilistic safety assessments.

1.2 Task and report organisation

The initial work plan for Task 2.2.E was defined in terms of five topics:

- Topic 1 – Identification of software needs and software development
- Topic 2 – Methodology and procedure
- Topic 3 – Sharing experience
- Topic 4 – Complementary calculations
- Topic 5 – The regulator's perspective

The work for these topics was distributed originally among Nagra, AF-Colenco (Switzerland), ENRESA (Spain) and Clausthal University of Technology, Institute of Disposal Research (Germany), with Nagra being the task leader.

Topic 1 is split into two parts that are covered in Chapters 2 and 3 of this report. Part 1, as summarised in Chapter 2, is dedicated to the first step in the development of the integrated PSA tools: Identifying the safety relevant features, events and processes (FEPs) which need to be modelled with the PSA tools. The corresponding process is described and the results are documented in the FEP-Screening Report (Milestone M2.2.E.2), which was published as Nagra Report NAB 07-38 (Nagra 2007). As there was no commercial software package that could cope with all the identified FEPs, new software had to be developed in the course of the project (Part 2 of Topic 1, summarised in Chapter 3). This part of Topic 1 focuses on the development of the components of the PSA tools, and on the design of appropriate interfaces between the components. The new software package is described in the Software Architecture Report (Milestone M2.2.E.3), which was published as Nagra Report NAB 09-35 (Nagra 2009a).

Topic 2 was originally intended to apply the PSA tools developed under Topic 1. However, after completion of the FEP-Screening Report it became clear that the development, implementation and application of a software package that would be capable of handling all identified FEPs simultaneously would be beyond the scope of the PAMINA Project. Consequently an alternative was developed; i.e. a simplified PSA modelling approach using a

set of existing tools. This simplified approach has the advantage of being more flexible and the disadvantage that not all the identified FEPs can be addressed. This simplified approach is described in Chapter 4.

Topic 3 encompasses a series of presentations at the final PAMINA Meeting. The corresponding presentations, which were given at the final PAMINA Meeting 2009 in Hohenkammer, Germany, are included in Appendix D of this report.

Topic 4 is about testing the ability of the radionuclide transport module of the probabilistic simulation software GoldSim to address specific issues from the list of requirements of the PSA as defined by Nagra. The data and scenarios are taken from Nagra's Project Opalinus Clay (Nagra 2002a). The results are published as Milestone Report M2.2.E.4 (ENRESA 2009) and presented in Chapter 5 of this report.

Topic 5, the regulator's perspective, is addressed in the Milestone Report M2.2.E.5 by Röhlig & Plischke (2009).

The organisation of the report is summarised in Table 1.2-1, below.

Tab. 1.2-1: Organisation of the present report.

Chapter	**Topic addressed**	**Contents**
1	-	Introduction
2	1	Identification of safety-relevant features, events and processes that the new PSA suite of codes should be able to represent
3	1	Software architecture foreseen for the new PSA suite of codes and development of its main component, the Integrated Radionuclide Release Code IRRC
4	2	Simplified PSA modelling using pre-existing Nagra codes (instead of the originally planned application of the PSA suite of codes developed under Topic 1)
5	4	Complementary (simplified) calculations using GoldSim RT, the commercially available radionuclide release and transport part of the GoldSim Package (ENRESA)
6	2, 4	Comparison of results from two independently performed simplified PSA calculations using (i) pre-existing Nagra codes and (ii) GoldSim RT
7	1, 2, 3, 4	Status, outlook and conclusions
8	-	References
Appendix A	-	List of abbreviations
Appendix B	-	HLW repository input parameters
Appendix C	-	L/ILW repository input parameters
Appendix D	3	Sharing experience (presentations given at the final PAMINA Meeting)

1.3 Starting point and methodology

The starting point for the development of the new PSA approach was the Safety Case prepared for Project Opalinus Clay, a demonstration of disposal feasibility of spent fuel (SF), vitrified high-level waste (HLW) and long-lived intermediate-level waste (ILW) in the Opalinus Clay in northern Switzerland (Nagra 2002a, b and c). The approach for the assessment of radionuclide release and transport was based on a combination of deterministic and probabilistic analyses.

The results from the deterministic analyses are relatively easy to understand and simple to explain, particularly to non-specialists. But, considering deterministic analyses only, the question remained whether unfavourable combinations of parameter values may have been overlooked. For that reason complementary probabilistic analyses were undertaken, which take into account combined effects of uncertainties. They provided assurance that no unfavourable combinations of parameter values existed that could compromise safety and that key contributors to uncertainty had been adequately addressed.

After the completion of Project Opalinus Clay, Nagra decided to strengthen the probabilistic approach and initiated a PSA development project in 2005. Phase 1 encompassed a Pilot Study (Nagra 2006) with an approach with certain limitations. In particular, the simultaneous and parallel modelling of all relevant phenomena was not possible. Phase 2 began in 2006 with the development of a probabilistic approach which considered all potentially relevant phenomena, including gas generation in the repository and gas transport through the engineered barrier system and the host rock. Nagra joined PAMINA with this project under the motto 'sharing experience'.

The essential first task in the project was the derivation of a comprehensive list of relevant phenomena to be modelled. To ensure that the broad range of uncertainties associated with potentially safety-relevant phenomena would be adequately considered in deriving such a list, it was viewed as important to get the scientists representing the various disciplines directly involved early on in the project through a clearly defined process. Consequently such a process was developed and applied to derive the list of relevant phenomena to be included in the PSA tools (see the FEP-Screening Report (Nagra 2007) mentioned above).

The second, and most ambitious, task of the project was to develop a software package capable of simultaneously modelling all the identified phenomena and their interactions. It was soon recognised that such a suite of codes may (initially) not run sufficiently fast for large numbers of probabilistic calculations. It was also recognised, however, that if this should turn out to be the case, then the codes may be successively simplified by exclusion of individual phenomena until the software package runs fast enough for PSA calculations. There are two key advantages of such an approach: (i) By comparing the results before and after an individual simplification, the effect of that simplification can be quantitatively assessed, and (ii) the effect of that simplification on computer run time can be quantitatively assessed. These two aspects of the simplification can be used to guide a decision as to which phenomena to include in probabilistic applications. Thus even using the tool in a deterministic mode can provide valuable insights into the effects of the individual phenomena.

The third task was to develop a set of corresponding independent complementary calculations using existing software tools (see Topic 4, above). This was done by two independent groups using independent software: (i) ENRESA and (ii) AF-Colenco.

The fourth task, a review of the regulatory situation regarding probabilistic safety assessments, was deliberately undertaken (and documented) independently from the PSA development work described above (see Topic 5, above).

2 Identification of safety relevant features, events and processes

A working group was established in August 2006 specifically for this FEP-screening task. The specialists included experts in safety analysis, radionuclide transport modelling, gas transport modelling, waste characteristics, geochemistry, geosciences, etc. If an identified FEP required special attention, new sub-groups with additional experts were formed to address this FEP, in some cases supported by complementary process modelling[1]. Ten expert meetings were held overall and documented in internal notes. The results are presented in the FEP-Screening Report (Nagra 2007).

The objective for this FEP-screening task was to identify and evaluate all potentially safety relevant phenomena and processes and their interdependencies as a preliminary step to the development of a new PSA tool. The working group followed a step-wise procedure.

The first step was to generate an unbiased list of all potentially safety-relevant FEPs. The selection was based on experience from earlier long-term safety assessments for radioactive waste repositories, but clearly focussed on a deep geological repository for spent fuel SF, vitrified high-level waste HLW, and long-lived intermediate-level waste ILW (and low- and intermediate-level waste L/ILW) in the Opalinus Clay formation. This starting list of 86 potentially safety-relevant FEPs is referred to as 'list of candidate FEPs' in Nagra (2007). In the reference document, each FEP is discussed with respect to its relevance to Swiss repository types and potential host rocks, process understanding, and an evaluation of the effect of the FEP.

In a second step, a judgement was made for each FEP in the 'list of candidate FEPs' on whether or not it should be included in the 'list of accepted FEPs'. In the end, the list of phenomena recommended to be modelled with the new PSA tool included 52 FEPs.

In summary, the evaluation of the phenomena encompassed:

1. Identification of potentially safety relevant phenomena for the 'list of candidate FEPs'
2. Discussion of the phenomena with respect to:
    - process understanding, evolution and possible consequences
    - relevance with regard to the Swiss repository types and host rock options[2]
    - the possibility to rate (or exclude) the phenomenon based on fundamental principles
3. Judgement on the impact on long-term safety and the inclusion in the 'list of accepted FEPs'

The accepted FEPs are compiled in two tables: Tab. 2-1 contains the environmental processes, i.e. processes acting to change the characteristics of the repository over time (without consideration of the release and migration of radionuclides). Tab. 2-2 lists the radionuclide processes, i.e. processes related to the release and migration of radionuclides within the repository system. Included are all processes judged to be safety relevant for the considered

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[1] Examples are FEPs concerning potential sealing effects of a high-pH plume in the host rock and the tunnel backfill.

[2] While the focus was on repositories in Opalinus Clay, options for L/ILW-type repositories in other potential host rocks were also evaluated. However, this supplementary information was not considered any further in the context of the IRRC model conceptualisation or the PSA project.

repository types and the Opalinus Clay host-rock option, under the conditions of the base scenario. These accepted FEPs and their interdependencies need to be taken into account by the standard or base version of the IRRC.

The list of accepted FEPs as it results from the FEP-screening process does not include any specifications of models or conceptual representations of the phenomena. Also, no criteria related to the feasibility or difficulty of implementing a phenomenon in a simulation model were applied in the evaluation. The sole criterion for screening-in a phenomenon into the 'accepted' list was the non-negligible potential impact on the long-term safety of deep geological repositories for SF, vitrified HLW, and ILW (and L/ILW) in the Opalinus Clay formation in Switzerland. The main information sources for the assessment were the findings from Nagra's Project Opalinus Clay (Nagra 2002a), and related published and unpublished reports.

Tab. 2-1: Summary of the environmental processes which are judged to be safety relevant.

Category	**FEP Nr.**	**Process (FEP)**	**Opalinus Clay SF/HLW**	**Opalinus Clay ILW & L/ILW**	**Remarks**
Hydraulic & Gas	1	Water flow through rock matrix	×	×	incl. fissures
	2	Water flow through transmissive discontinuities in host rock	×	×	incl. channelling
	3	Gas/water flow through EDZ	×	×	
	4	Gas/water flow through sealing zones	×	×	bentonite & sealing zone EDZ
	5	Gas/water flow through concrete backfill		×	between emplacement tunnel and operations tunnel
	6	Water flow in confining units	×	×	excluding regional aquifers
	7	Resaturation of cementitious backfill		×	evolution of gas pressure depends on initial saturation
	8	Gas generation by anaerobic corrosion of metals, microbial degradation, radiolysis, and decay	×	×	
	9	Effective water consumption by gas generation	×	×	
	10	Gas dissolution / degassing	×	×	
	11	Formation of gas phase and gas pressure build-up	×	×	

Tab. 2-1: (Cont.)

Category	FEP Nr.	Process (FEP)	Opalinus Clay SF/HLW	Opalinus Clay ILW & L/ILW	Remarks
Hydraulic & Gas	12	Gas-induced porewater displacement	×	×	little porewater displacement in bentonite; Figure 7.4-7 in Nagra (2002a)
	13	Gas transport by advection / diffusion of dissolved gas	×	×	
	14	Gas transport by two-phase flow	×	×	capillary flow; Figure 3.1-1 in Nagra (2004), Picture 2
	15	Gas transport by dilatant gas pathway formation	×	×	reversible; Figure 3.1-1 in Nagra (2004), Picture 3
	16	Gas accumulation in confining units	×	×	hydraulics / release of volatile ^{14}C along gas pathway
	17	Rock mechanical evolution of EDZ	×	×	decreasing hydraulic conductivity and gas permeability
Mechanical	18	Tunnel convergence		×	displacement of porewater
	19	Increase of hydraulic conductivity by uplift / erosion	×	×	decompaction, transient flow field
	20	Chemical / mineralogical alteration of bentonite	×		by iron, cement, high pH plume etc., increase of hydraulic conductivity
Chemical & Microbial	21	High-pH plume: sealing effect in host rock		×	by iron, cement, high pH plume etc., increase of hydraulic conductivity
	22	Anion exclusion	×	×	
	23	High-pH plume: tunnel backfill sealing effect		×	

Tab. 2-2: Summary of the radionuclide processes which are judged to be safety relevant.

Category	**FEP Nr.**	**Process (FEP)**	**Opalinus Clay SF/HLW**	**Opalinus Clay ILW & L/ILW**	**Remarks**
Radioactive inventory and decay	24	Partitioning of inventory	×	×	IRF, cladding, matrix: for SF and part of ILW; STMAN
	25	Speciation of radionuclides	×	×	considered in solubility and sorption databases
	26	Speciation of ^{14}C	×	×	3 fractions of ^{14}C: inorganic dissolved, organic dis-solved, organic in the gas phase
	27	Chain decay	×	×	branching, ingrowth
Containment failure mechanisms	28	Breaching of canisters	×		STMAN
	29	Pinhole defects of canisters	×		and resistance; STMAN
	30	Breaching of waste containers		×	STMAN (ILW)
Radionuclide mobilisation	31	Glass dissolution	×		STMAN (HLW)
	32	Cladding corrosion	×	×	STMAN (SF/ILW/ cladding)
	33	Leaching of IRF	×	×	STMAN (SF/ILW)
	34	Fuel matrix dissolution	×		STMAN (SF)
	35	Radionuclide release from cemented and / or metallic wastes		×	STMAN (ILW)
	36	Precipitation of radionuclides	×	×	incl. isotopic dilution, relevant for near field transport only; STMAN
	37	Corrosion products – redox effects	×	×	considered in solubility and sorption databases

Tab. 2-2: (Cont.)

Category	FEP Nr.	Process (FEP)	Opalinus Clay SF/HLW	Opalinus Clay ILW & L/ILW	Remarks
Radionuclide mobilisation	38	Advection / dispersion	×	×	
	39	Diffusion	×	×	
	40	Matrix diffusion	×	×	only in connection with transmissive features (fractures)
	41	Sorption	×	×	
	42	Facilitated transport by complexing agents	×	×	considered by sorption database
Transport of volatile radionuclides (^{14}C)	43	Advection / dispersion in gas phase	×	×	for SF, ILW and L/ILW
	44	Advection / dispersion of dissolved volatile radionuclides in the liquid phase	×	×	for SF, ILW and L/ILW
	45	Diffusion of dissolved volatile radionuclides in the liquid phase	×	×	for SF, ILW and L/ILW
	46	Diffusion of volatile radio-nuclides in the gas phase	×	×	for SF, ILW and L/ILW
	47	Dissolution / degassing	×	×	for SF, ILW and L/ILW
Radionuclide pathways through host rock and confining units	48	Transport through dilatant pathways	×	×	refers to FEP Nr. 15; includes matrix diffusion into adjacent rock matrix
	49	Transport through transmissive discontinuities	×	×	refers to FEP Nr. 2; includes matrix diffusion into host rock, not including FEP Nr. 48
	50	Transport through rock matrix	×	×	refers to FEP Nr. 1; rock matrix treated as equivalent porous medium

Tab. 2-2: (Cont.)

Category	**FEP Nr.**	**Process (FEP)**	**Opalinus Clay SF/HLW**	**Opalinus Clay ILW & L/ILW**	**Remarks**
Radionuclide pathways through access tunnel systems	51	Transport through / around sealing zones	×	×	transport through seals and EDZ around sealing zones
	52	Transport within backfill and EDZ	×	×	transport along tunnels with sand / bentonite backfill and EDZ; incl. matrix diffusion into host rock

3 Software architecture and development of the Integrated Radionuclide Release Code IRRC

This chapter gives a condensed summary of the software architecture foreseen to implement Nagra's probabilistic safety assessment (PSA) concept. It is based on the Software Architecture Report (Nagra 2009a), to which the reader is referred for additional information. The focus of the chapter is on the development of the IRRC, which was by far the most ambitious part of the code development work for this project.

3.1 Software architecture

After the safety-relevant FEPs to be considered had been identified (Chapter 2), the next step in the implementation of the PSA modelling approach was to develop a (deterministic) suite of codes that would be able to address all of the identified FEPs. This suite of codes, termed *Integrated Radionuclide Release Code IRRC*, would then be embedded in an environment that allows PSA calculations to be made (see Fig. 3.1-1). The key components of the IRRC are (i) the *Integrated Flow Code IFC* and (ii) the *Radionuclide Transport Codes RTC* STMAN-TD, PICNIC-TD and the Gas Model (see Fig. 3.1-2).

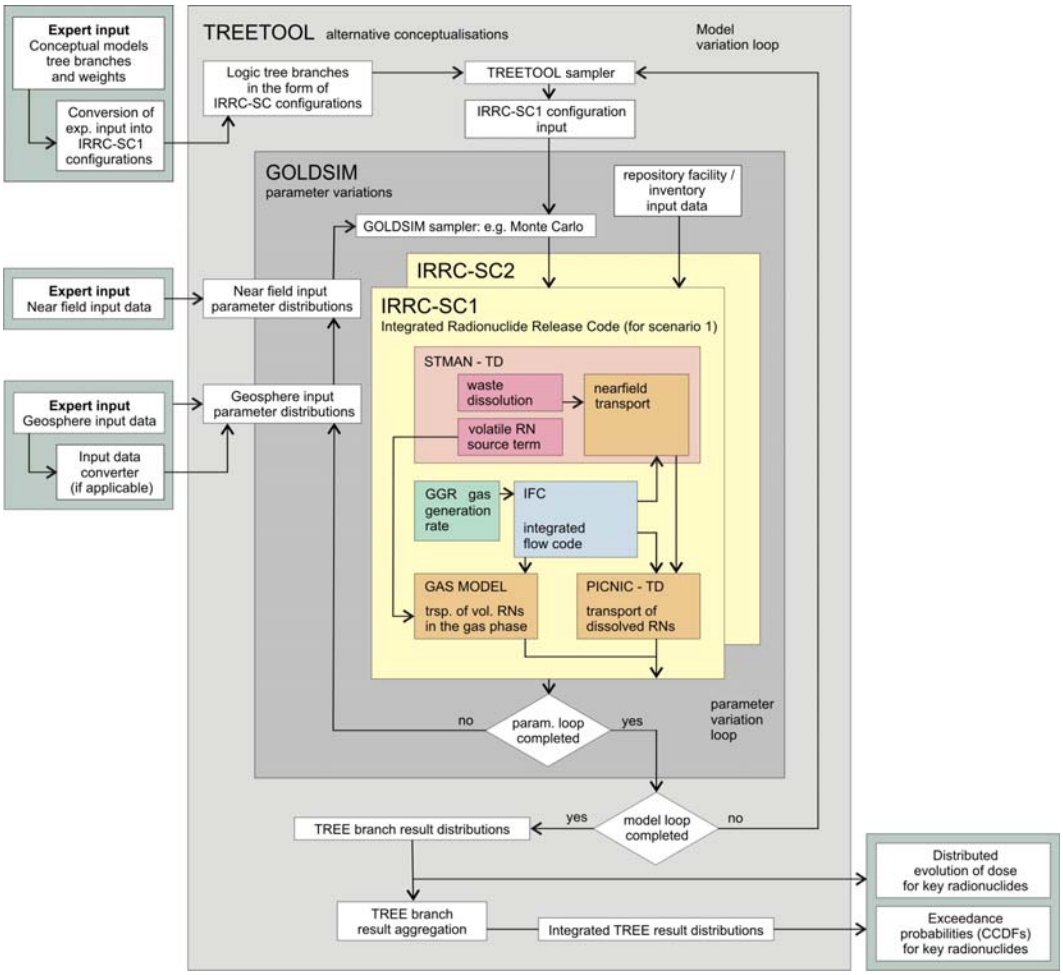


Fig. 3.1-1: Software architecture foreseen to implement Nagra's PSA concept.

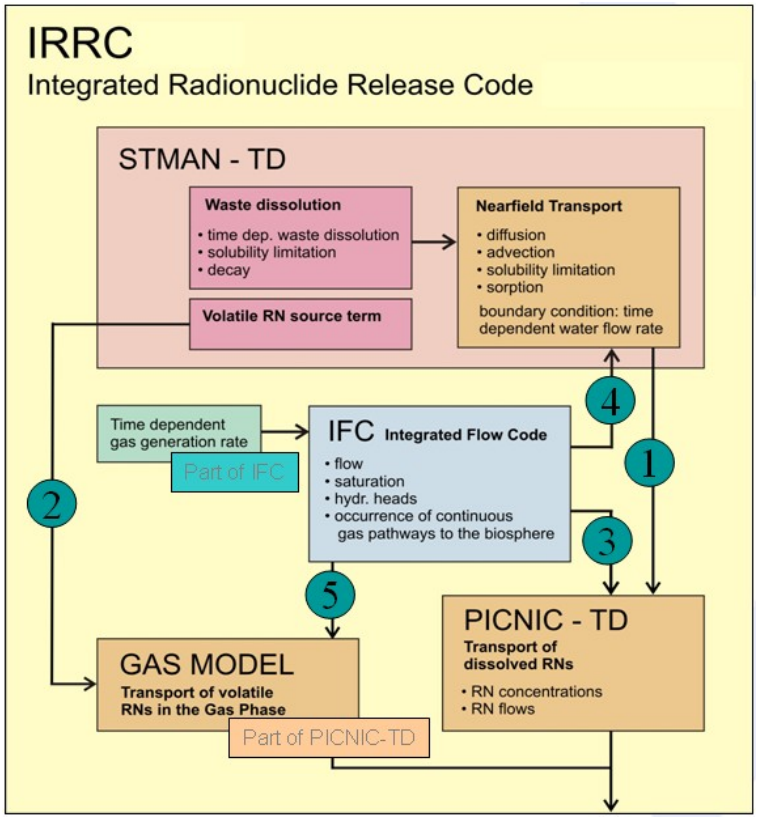


Fig. 3.1-2: Constituent codes and linkages between codes in the current implementation of the IRRC.

Codes: STMAN-TD, PICNIC-TD (with (simplified) Gas Model) and IFC.

Linkages: 1: STMAN-TD to PICNIC-TD; 2: STMAN-TD to Gas Model;
3: IFC to PICNIC-TD; 4: IFC to STMAN-TD; 5: IFC to Gas Model

As indicated by arrows 3, 4 and 5 in Fig. 3.1-2, the IFC, which calculates the time-dependent two-phase flow in the near field and geosphere of a gas-generating nuclear waste repository, passes on its flow results to the RTC suite of codes STMAN-TD, PICNIC-TD and the Gas Model, which calculate radionuclide releases from the repository system to the biosphere. Doses are then calculated using Biosphere Dose Conversion Factors (BDCFs, see Nagra (2002b) for a definition) for a given biosphere type (not shown in Fig. 3.1-2).

The IFC (Nagra 2009a) was developed specifically for Nagra's PSA project. The updated version of STMAN (Nagra 2009b), named STMAN-TD in Fig. 3.1-2, and PICNIC-TD (Nagra 2010) are variants of pre-existing radionuclide release and transport codes allowing for time-dependent ("TD") flow fields. STMAN-TD and PICNIC-TD were also developed specifically for Nagra's PSA project. The Gas Model calculates transport of volatile radionuclides in the gas phase. All component models are discussed further in Chapter 3.2, below.

The IRRC can be regarded as a deterministic code that can simultaneously take into account all 52 safety-relevant FEPs identified in Chapter 2 and explicitly listed in Tables 2-1 and 2-2. As indicated in Chapter 1.3, a first test version of the IRRC was successfully developed within the PAMINA Project, but this test version did not run sufficiently fast for probabislistic calculations. First results of the "stand-alone" IRRC running in deterministic mode are presented in Chapter 3.3.

A probabilistic driver such as GoldSim will be used to generate samples for the PSA calculations, indicated by the dark grey box labelled "GOLDSIM" surrounding the yellow IRRC boxes in Fig. 3.1-1. This is not discussed further in the present report.

To handle alternative, mutually exclusive conceptualisations (termed "scenarios" in Fig. 3.1-1), a logic tree approach will be used, indicated by a light grey box labelled "TREETOOL" surrounding the dark grey box labelled "GOLDSIM" in Fig. 3.1-1. This is not discussed further in the present report.

3.2 Development of the Integrated Radionuclide Release Code IRRC

As mentioned in Chapter 3.1, the key components of the IRRC are (i) the *Integrated Flow Code* (IFC) and (ii) the *Radionuclide Transport Codes* (RTC) STMAN-TD, PICNIC-TD and the Gas Model. These are discussed below.

The *Integrated Flow Code* is both a *numerical code* and a *model* of a specific HLW repository system based on that presented in Nagra's Project Opalinus Clay (Nagra 2002a). Details of both the numerical code and of how the model is implemented are given in the Software Architecture Report (Nagra 2009a). The IFC calculates the time-dependent water and gas flow fields in the repository system. The environmental processes listed in Table 2-1 are either directly simulated using (simplified) process models integrated in the IFC (e.g. the formation of dilatant gas pathways) or considered by using effective parameters calculated by separate process models (e.g. time-dependent gas generation rates).

The *numerical code* is a modification of the multiphase, multicomponent simulator TOUGH2 (Pruess et al. 1999), as implemented within the iTOUGH2 framework (Finsterle 2007a, b and c). The code modifications mainly involve the implementation of relevant FEPs as listed in Table 2-1, as well as removal of FEPs that are not needed.

The *model* is a simplified representation of the repository system. Specifically, a computational grid was generated, which includes the emplacement tunnels for spent fuel, vitrified HLW and long-lived intermediate-level waste. Moreover, the model represents engineered barriers (backfill, seals, plugs, etc.), various tunnels and other underground facilities, and includes a simplified representation of the geological structure, i.e., the host rock (including the excavation disturbed zone (EDZ) around the underground openings), confining units, local aquifers, and a highly-transmissive zone.

The *Radionuclide Transport Codes* encompass STMAN-TD, PICNIC-TD and the Gas Model.

STMAN-TD (Nagra 2009b) is a further development of STMAN, a previously existing Nagra tool for modelling radionuclide release and transport in the near field. It deals with three possible sources of radionuclides: Spent fuel, vitrified HLW and long-lived intermediate-level waste. Within the context of the integration of STMAN in the IFC, a number of enhancements to STMAN have been made, which lead to the release of a new version, 5.7.2, named STMAN-TD in the present report. The main objective of the modifications was to enable STMAN-TD to

deal with time-dependent groundwater flow rates, which can be read in from files generated by the IFC.

PICNIC-TD (Nagra 2010) is a geosphere transport code that has been developed specifically for Nagra's PSA project. The concept is based on PICNIC, a previously existing Nagra tool for modelling radionuclide transport in the geosphere. PICNIC-TD can deal with time-dependent groundwater flow rates, which can be read in from files generated by the IFC. PICNIC-TD is a general-purpose code, appropriate for both fractured and porous systems. The system modelled by PICNIC-TD consists of a network of one-dimensional transport legs, each representing a section of the pathways through the geosphere. In terms of the network, the basic concepts are legs and junctions. Every leg has an upstream end and a downstream end, each corresponding to a particular junction. In PICNIC-TD there is assumed to be full coupling between the legs that meet at a junction, through a shared concentration. This differs from the earlier PICNIC code (Robinson 2004), where it was assumed that each leg was advectively dominant, so that there was no feedback from downstream legs on their upstream precursors. This coupling at junctions makes PICNIC-TD more suitable for diffusively-dominated systems than PICNIC. PICNIC-TD uses spatial discretisation and a time-stepping solver, rather than the semi-analytic Laplace-transform approach used in PICNIC.

The Gas Model, in the current version of the IRRC, is a simplified version which assumes direct transfer of the volatile radionuclides in the gas phase to the biosphere aquifer if continuous gas paths to the biosphere are present. Whether this is the case or not is calculated for each realisation by the IFC.

The IRRC is in principle ready for use. Deterministic test calculations have shown the correctness of the implementation. However, the development was more difficult than had been anticipated. The computational time required by the IFC for a complete repository model including all safety-relevant FEPs is currently too high for probabilistic calculations. Therefore, the IRRC is at present used as a research tool helping to understand the complex processes involved (see also the discussion in Chapter 7).

3.3 Experience with first applications of the IRRC and first results

Within the IRRC, the IFC needs most of the computing time. The maximum version that explicitly considers all safety-relevant FEPs (see Chapter 2) is relatively slow. The maximum CPU time[3] required for the IFC, with all safety-relevant FEPs included, is about 45 hours for a 1 million year period (solid curve in Fig. 3.3-1). The CPU time required decreases to about 15 hours for a 1 million year period if the five "special FEPs" listed in the figure caption of Fig. 3.3-1 are excluded (dot-dashed curve in Fig. 3.3-1).

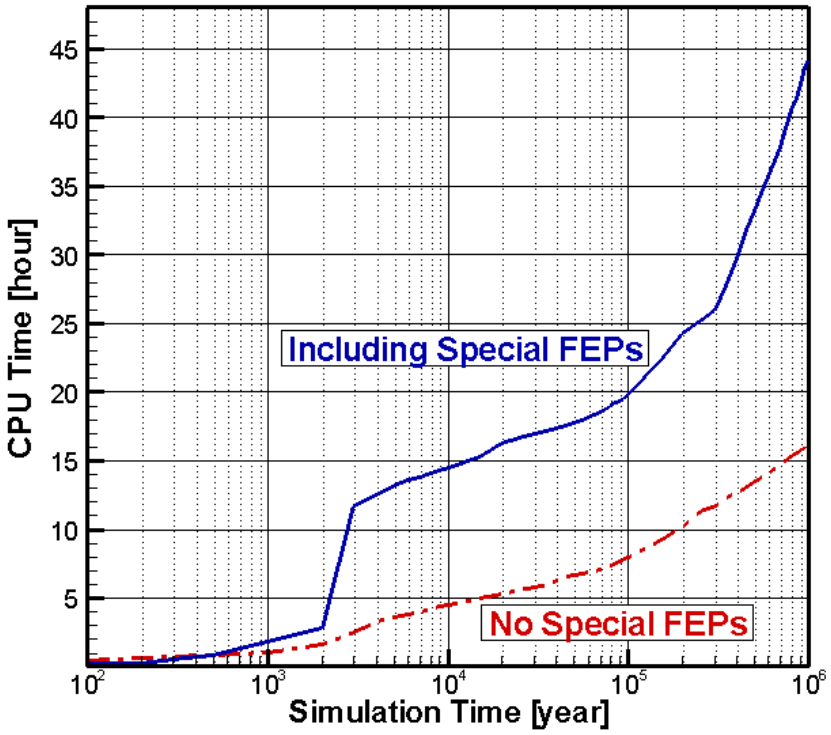


Fig. 3.3-1: CPU time as a function of simulation time for a IFC simulation with and without the inclusion of geomechanical and geochemical FEPs.

The solid curve (blue) represents a simulation with all safety-relevant FEPs included. In the simulation represented by the dot-dashed curve (red), the following FEPs have been excluded: (i) pathway dilation, (ii) EDZ self-sealing, (iii) tunnel convergence, (iv) uplift/erosion, (v) geochemical sealing. From Nagra (2009a).

[3] The simulation was performed on a Dell laptop, Latitude D620, with an Intel© Corel™ 2 CPU T7600 @ 2.33 GHz and 2 GB of RAM, running under Microsoft Windows XP, Professional, Version 2002, Service Pack 3. The FORTRAN source code was compiled using the Intel® Visual FORTRAN Compiler 9.1.

All other IRRC calculations (i.e. the radionuclide release and transport calculations) take about 40 minutes with all radionuclide processes being considered. This applies to a case with a network of 36 PICNIC "legs" representing radionuclide transport in the underground structures, in the backfilled and sealed access ramp and shaft and through the host rock and confining units and considering 39 nuclides (see Fig. 3.3-2). If matrix diffusion from the tunnels into the host rock is neglected, the required CPU time is reduced to about 8 minutes; if in addition longitudinal flow in the tunnels is neglected, a further reduction to about 3 minutes is observed. The effect of these simplifications on calculated doses are negligible.

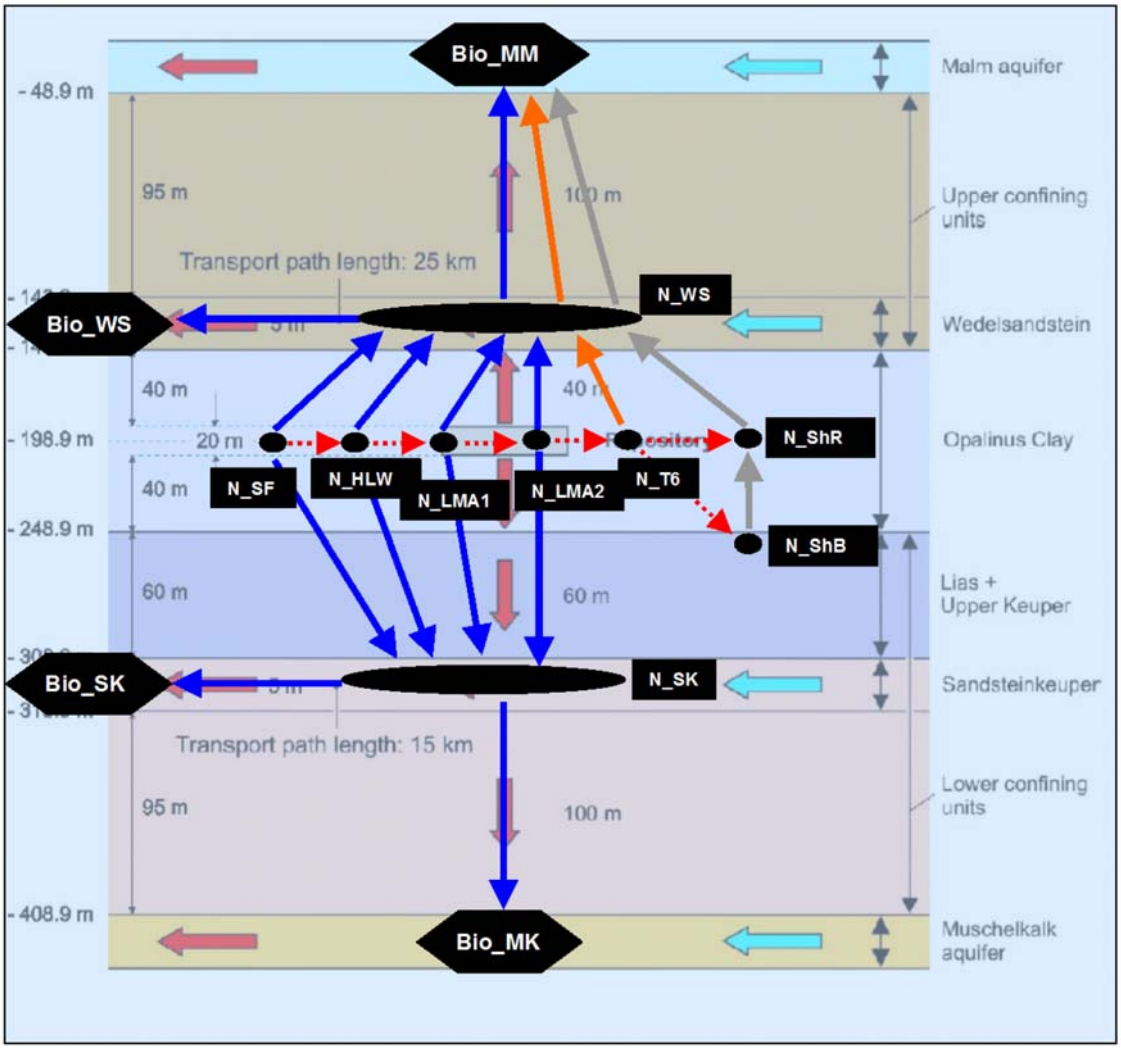


Fig. 3.3-2: IRRC network with 36 PICNIC "legs" (vertical cross section).

Red legs: transport in tunnels (excluding emplacement tunnels; these are shown as black dots in this vertical cross section)

Orange legs: transport in access ramp

Grey legs: transport in shaft

Blue legs: transport in host rock and confining units

Fig. 3.3-3 shows an example result from the IRRC for the network of 36 PICNIC "legs" described above with all safety-relevant FEPs included. The flow field used by the radionuclide transport codes was calculated by the IFC using the base case parameter values as given in Nagra (2009a). The radionuclide process related geosphere transport parameters used by the radionuclide transport codes correspond to the reference case values from Project Opalinus Clay (Nagra 2002a). The result is expressed in terms of a hypothetical dose obtained by converting radionuclide release from the Opalinus Clay into the Wedelsandstein in the upper confining units above the host rock Opalinus Clay (see Fig. 3.3-2) by multiplying the releases by the Biosphere Dose Conversion Factors (BDCFs) for the Reference-Case biosphere in Project Opalinus Clay (Nagra 2002a, Tab. A2.11).

A number of observations can be made regarding this example result. First, it is noted that the maximum of the (hypothetical) dose is about 7×10^{-5} mSv/a, i.e. more than three orders of magnitude below the Swiss regulatory protection criterion of 0.1 mSv/a. This is comparable to the calculated reference case dose maximum in Project Opalinus Clay, which was 5×10^{-5} mSv/a (Nagra 2002a). However, a direct comparison may not be very meaningful since the IRRC is quite different from the suite of codes used to calculate the reference case results in Project Opalinus Clay. Nevertheless, it is remarkable that the results from the IRRC, with 52 safety-relevant FEPs explicitly included, yields similar results as the reference case of Project Opalinus Clay. It is pointed out that "expected" doses would be substantially lower than those shown since the radionuclide transport distances to the exfiltration points to biosphere aquifers are large, with a corresponding further reduction in dose due to additional radionuclide decay and dispersion. In Project Opalinus Clay, lateral transport distances in the Wedelsandstein and in the Sandsteinkeuper were given as 25 km and 15 km, respectively. Additional vertical transport distances upward to the Malm aquifer and downwards to the Muschelkalk aquifer are of the order of about 100 m each; with similar favourable radionuclide retention properties as the host rock Opalinus Clay (Nagra 2002a).

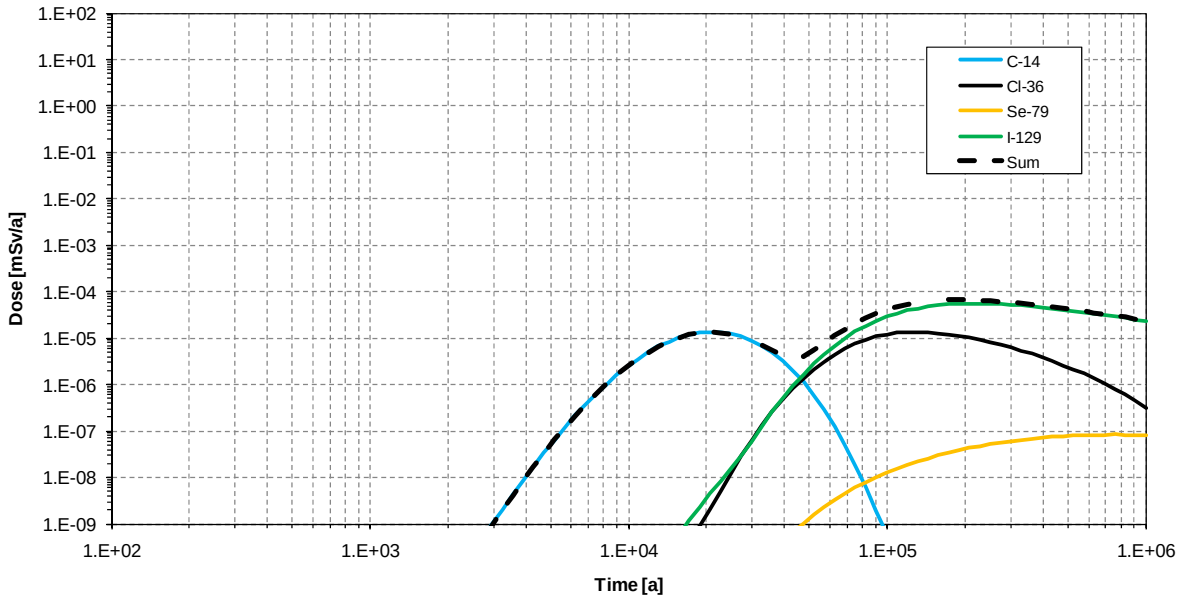


Fig. 3.3-3: Example of an IRRC result for a network with 36 PICNIC "legs" with all 52 safety-relevant FEPs included (sum of contributions from SF, HLW and ILW).

See text for details.

4 Simplified PSA modelling using pre-existing Nagra codes

Since the development of the IRRC was more difficult and time consuming than originally thought, Nagra decided to follow a second path (parallel to the development of the IRRC); i.e. the development of a simplified modular PSA tool using the same Monte-Carlo simulation software GoldSim (GoldSim Technology Group 2009) as foreseen to perform probabilistic calculations with the IRRC. This simplified tool should be suitable for modelling radionuclide release and transport for a HLW repository. In addition, to make use of synergies, it was decided to develop an analogous tool in parallel suitable for modelling a low- and intermediate-level waste (L/ILW) repository. The simplified PSA tools should make use of Nagra's existing palette of deterministic modelling tools for radionuclide release and transport, namely of the codes STMAN, VPAC and PICNIC. Fig. 4.1-1 illustrates this simplified PSA modelling approach.

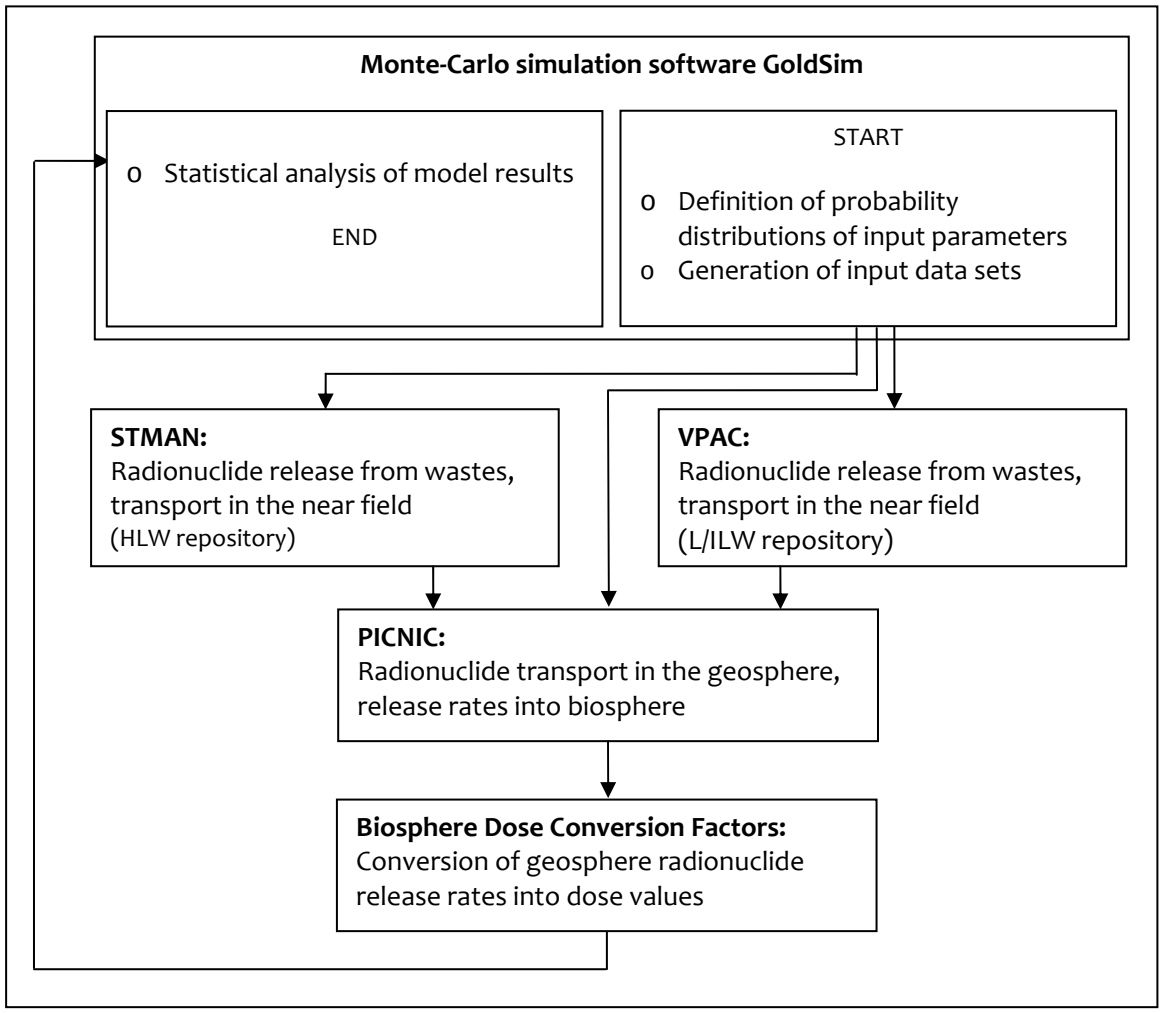


Fig. 4.1-1: Codes used in the simplified PSA modelling approach.

In the present chapter, the numerical tools used for the simplified PSA modelling approach and their connectivity are introduced, and results of first test applications of the simplified PSA modelling approach are presented both for a generic HLW repository and a generic L/ILW repository[4].

4.1 Tools

4.1.1 GoldSim

GoldSim is a graphical, Windows-based program for carrying out dynamic, probabilistic simulations (GoldSim Technology Group 2009). Originally developed for radioactive waste management and mining projects, GoldSim is a flexible and general-purpose stochastic modelling environment with a broad range of potential applications including business modelling, engineered systems modelling and environmental modelling. Furthermore, GoldSim offers add-on modules for specific problems such as reliability and maintenance calculations or contaminant transport. Of special interest for PAMINA is the radionuclide transport module of GoldSim, which is the basis for the probabilistic calculations presented in Chapter 5. In the simplified PSA modelling approach discussed here, GoldSim is used as Monte-Carlo simulator that handles the probabilistic input and output management of the different external radionuclide transport codes for the near field and geosphere calculations. GoldSim allows the coupling of external program modules via DLLs (Dynamic Link Libraries). For the simplified PSA, an interface between GoldSim and the programming language Python was developed. This C-coded DLL allows GoldSim to call Python functions and facilitates the embedding of external programs via Python scripts.

4.1.2 STMAN

STMAN is a source term performance assessment modelling code for the near field transport and decay of radionuclides released from repositories. It deals with three possible sources of radionuclides: high-level vitrified waste, low-level cementitious waste and spent fuel rods. These different sources are dealt with by the STRENG, STALLION and SPENT options respectively. For each of the source term models (STRENG, STALLION and SPENT) the repository may be surrounded by a bentonite buffer. Within this buffer, the processes of diffusion, sorption and radioactive decay take place. Solubility limits within this region may be defined, and an inner and outer region that may have different properties may be specified. Radionuclides that pass through the bentonite buffer are carried away. The following short descriptions are a summary of Nagra (2009b).

The STRENG source term model is used for high level waste, held in a vitrified matrix, within a canister. The nuclides are released as a result of glass dissolution, following the failure of the surrounding metallic canister at a time specified by the user. The STRENG model assumes cylindrical symmetry as shown in Fig. 4.1-2.

The SPENT source term model assumes that the source of radionuclides is a number of spent fuel rods in a spent fuel canister. Each fuel rod is assumed to contain a fractured matrix of fuel. The radionuclides are distributed in three regions within the fuel: in the fuel matrix, at grain boundaries and within the gaps. For both STRENG and SPENT, at some specified time, the canister is assumed to fail completely. From that point onwards, the fuel is assumed to be surrounded by water forming a reservoir into which the radionuclides may be released.

[4] For the allocation of waste types to these repositories, the reader is referred to Nagra (2008a).

Radionuclides in the fuel gaps and grain boundaries are assumed to be released immediately into the reservoir, whilst others, in the matrix, are released at different, controlled rates.

The STALLION source term model is used for low or intermediate level waste in either a cylindrical or spherical geometry as shown in Fig. 4.1-2. The radionuclides in the repository are initially held in a dry, porous cement matrix inside a thin steel canister (treated as infinitesimally thin). A bentonite buffer may optionally be considered. At a specified time the canister is assumed to have failed and to no longer present a barrier to the diffusion of radionuclides into the bentonite and/or the host rock. Some fraction of the radionuclide inventory is assumed to be embedded in solid metal form and to be slowly released. The remaining inventory is immediately available for release.

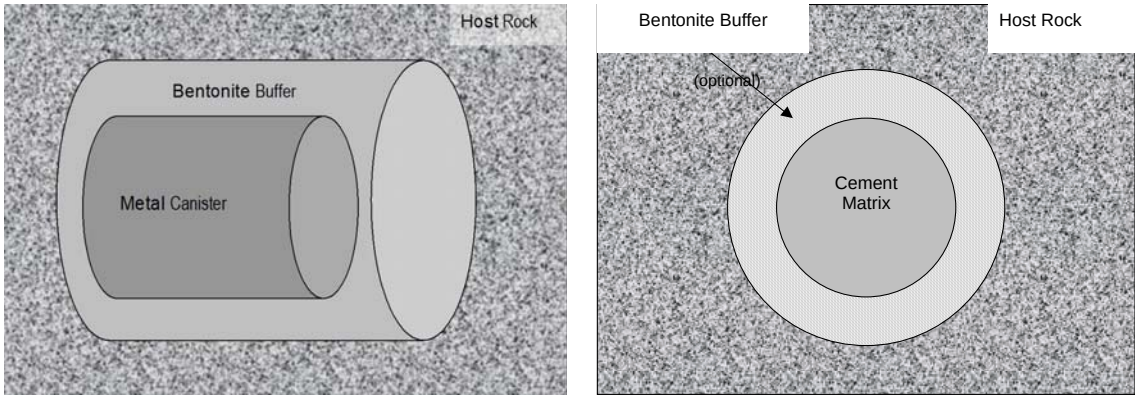


Fig. 4.1-2: The geometry of a high-level waste canister containing vitrified HLW (left) and of a low or intermediate level waste tunnel with cementitious waste forms (right).

In its current version (named STMAN-TD in Fig. 3.1-1), STMAN allows for the use of time-varying groundwater flow rates. For the simplified PSA presented in this chapter, only steady-state flow conditions have been applied.

4.1.3 VPAC

The *Versatile Performance Assessment Code* (VPAC) is a numerical code that simulates groundwater flow and radionuclide release and transport in fully saturated heterogeneous media (Nagra 2008b). The flow and transport equation systems are approximated using the Mixed-Hybrid Finite Element Method. The code can handle one-, two- and three-dimensional problems. It has the following modelling capabilities:

- Stationary and instationary saturated flow
- Radionuclide transport by advection, dispersion and diffusion
- Radioactive decay and ingrowth for an unlimited number of radionuclides and unlimited decay chain lengths
- Solubility limitations
- Instantaneous and / or time-dependent, geometry-dependent radionuclide release (e.g. due to corrosion of activated steel)
- Time-dependent hydraulic conductivity

- Time-dependent diffusion
- Time-dependent sorption

VPAC is an integrated tool for flow and transport both in the near field and in the geosphere. It is suitable for SF and HLW as well as for ILW and L/ILW. It combines the ability to model the full range of radionuclide release and transport processes mentioned above with the possibility to directly calculate radionuclide fluxes along arbitrarily defined interfaces within the model domain.

The model parameters defining the fluid flow in a simulation are assigned to "material classes" in VPAC. These material classes can be associated with different hydraulic or geological units and are assigned to the cells of the FE-mesh used. Transport parameters such as sorption coefficient, diffusion coefficients and solubility limits usually vary for different chemical elements. Therefore these parameters can be defined individually for each chemical element and each material class. Radionuclide-specific data such as half-life are specified for each nuclide in the VPAC input files.

In the present study VPAC is employed to model the radionuclide near field release from L/ILW that serves as model input for the geosphere transport calculations with PICNIC (see below).

4.1.4 PICNIC

PICNIC models the transport of radionuclides in the geosphere. While PICNIC-TD can handle time-variable flow fields (see Chapter 3), its precursor PICNIC assumes steady-state flow conditions. The simplified PSA presented in this section had been performed without taking credit of non-steady flow conditions. The following description is a summary of Robinson (2004).

A system represented by PICNIC consists of a network of one-dimensional transport paths (called legs in PICNIC), each representing a section of the pathways through the geosphere. The structure of this network may be based on analysis of a continuum flow model or a discrete fracture network model, or it may be directly created by the user. In terms of the network, the basic concepts are legs and junctions. Every leg has an upstream end and a downstream end, each corresponding to a particular junction. Junctions can have several incoming and outgoing legs. Some junctions have no incoming legs, but are connected to a source term. Some junctions have no outgoing legs, but produce a "result". Legs may have additional diagnostic outputs (e.g. total mass in leg). Fig. 4.1-3 illustrates a possible network, with the different types of junction that can arise.

It is assumed that each leg is advectively dominant, so that there is no feedback from downstream legs on their upstream precursors, and thus the network has definite paths through it. The important consequence of this assumption is that the network system can be solved by assembling solutions for each individual leg. Each leg can determine its output (generally a mass flux at its downstream end) once its input (mass flux at the upstream end) is given. Thus the network consists of legs which transform their inputs to give their outputs. The connected structure of the network is used to impose mass flux conservation at the junctions.

Each leg has some properties specific to itself and others derived from an associated rock-type. Each rock-type can be linked to any number of legs. Rock-types consist of flow and matrix components. The individual leg properties include its location and length. Flow and matrix

properties include porosity and retardation or retention. The retardation and matrix-retention can either be set directly or calculated from basic physical parameters including porosities and sorption coefficients.

The PICNIC code handles decay, including splitting and joining chains and ingrowth, with the supplied decay details being used to produce a set of linear decay chains. All the parameters within the PICNIC network, including physical and chemical properties, are restricted to being time-invariant, and the processes modelled are linear in the mathematical sense. This allows the effect of each leg to be determined using a response function which is convoluted with the input to produce the output from the leg.

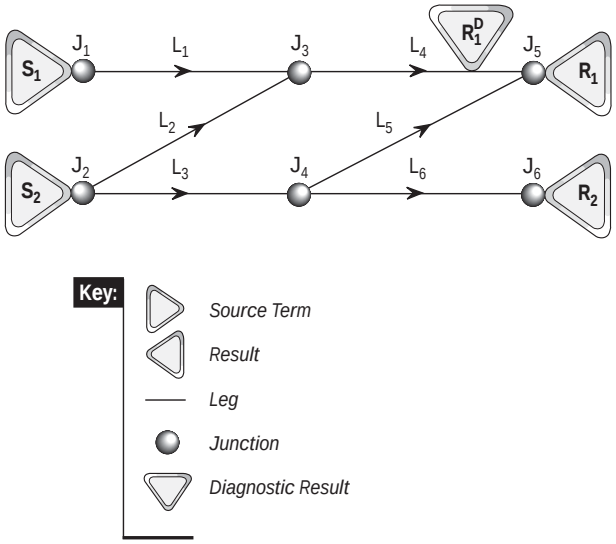


Fig. 4.1-3: An example PICNIC network.

4.1.5 Biosphere dose conversion factors

To convert calculated near field or geosphere releases into dose, steady-state biosphere dose conversion factors (BDCFs) were used as described in Nagra (2007). The biosphere compartment model TAME used in Project Opalinus Clay is transient, in that it explicitly takes account of the timescales of various phenomena resulting in the transfer of radionuclides between compartments. Since it is reasonable to assume that these timescales are short in comparison to the timescales over which releases from the Opalinus Clay vary significantly, simple BDCFs are to be derived, which are multiplied by releases from the Opalinus Clay in order to calculate doses. BDCFs are obtained by the following procedure: For each radionuclide *j*, a constant flux of 1 Bq/a is input into the transient compartment model, with the Reference Case conceptual assumptions (see Chapter 4.2.1) and parameters, and the model is run until a steady state is reached. The BDCF for radionuclide *j* is the ratio of the corresponding steady-state annual dose [mSv/a], summed over all daughter radionuclides, to the input value of 1 Bq/a. Doses calculated by multiplying the release from the Opalinus Clay of a particular radionuclide by its BDCF thus include the contributions of all its daughters. The reference case BDCFs are given in Tab. B-19 in Appendix B.

4.1.6 Presentation of results

Results are presented as

- median dose, 95th and 5th percentiles and highest / lowest dose maxima of all realisations as a function of time
- complementary cumulative distribution functions (CCDFs)
- maximum dose for each realisation and moving average as a function of realisation number
- parameter correlation with maximum peak dose
- mean dose as a function of time

For SF, HLW and ILW the time period of assessment is 10^6 years; for L/ILW it is 10^5 years (Nagra 2008a). Nevertheless, in the present report results are displayed up to a time of 10^7 years for both repository types, even though the assumptions made for the time period of assessment may not be valid any more at times beyond the period of assessment.

4.2 Application for a repository for HLW

4.2.1 Conceptual model and data

This project considers a repository sited in the Opalinus Clay of the Zürcher Weinland region in northern Switzerland that is designed for the disposal of:

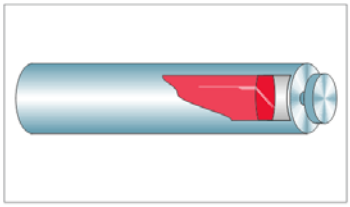
- spent fuel (SF), in the form of fuel assemblies containing UO2 or mixed-oxide (MOX) fuel,
- vitrified high-level waste (HLW) from the reprocessing of spent fuel, and
- long-lived intermediate-level waste (ILW).

The reference conceptualisation is that of the Reference Case of the Project Opalinus Clay as presented in Nagra (2002a and b). The related principal safety barriers are exemplified for HLW in Fig. 4.2-1.

Safety barrier system for HLW

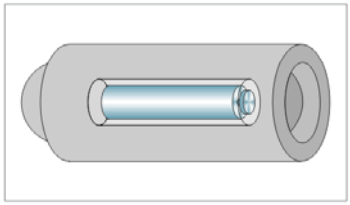
Waste matrix (glass)

- Fixation of radionuclides in the glass matrix
- Low glass corrosion rate



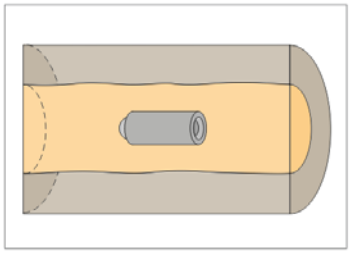
Disposal container

- Containment of the waste for several thousand years
- Thereafter: Restricted water inflow and retention of radionuclides (sorption on corrosion products)



Backfill (bentonite)

- Suitable interface between disposal containers and the host rock
- Favourable radionuclide retention properties
- Favourable conditions for long-term stability of the disposal containers



Host rock

- Low groundwater flux
- Favourable structure of the pore space
- Favourable geochemical conditions for radionuclide retention
- Favourable conditions for long-term stability of the engineered barriers

Geological situation

- Favourable host rock configuration for arrangement of the disposal tunnels
- Favourable conditions for long-term stability of the barrier system
- Absence of raw materials deposits that would be workable in the foreseeable future

Placement of disposal tunnels deep underground

- Isolation of the waste
- Prevention of unwanted access
- Protection from unintentional intrusion
- Protection from erosion

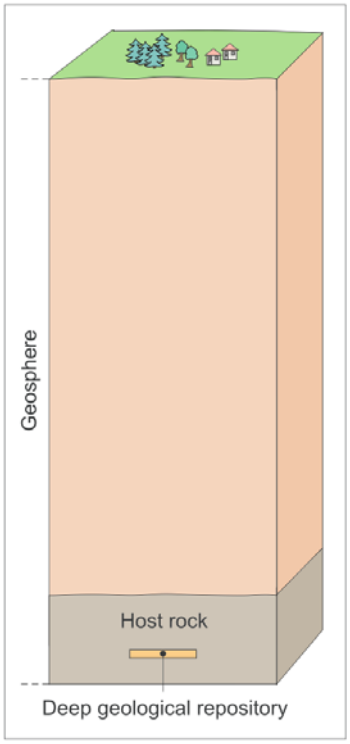


Fig. 4.2-1: The system of safety barriers in the case of vitrified HLW.

The Reference Case is based on a number of assumptions regarding the conceptualisation for modelling purposes of key FEPs associated with the various system components (the Reference Conceptualisation) together with a reference set of parameters. In the definition of the Reference Conceptualisation and reference parameter set, some pessimistic or conservative conceptual assumptions (and related parameter values) are used:

Spent fuel:

- The instant release fraction (IRF) is released from SF immediately upon canister breaching.
- Other radionuclides in the SF are released congruently with fuel matrix dissolution, at a time-dependent rate proportional to the α activity of the fuel.
- All ^{14}C originating from SF, including the IRF, is assumed to be in inorganic form. All ^{14}C originating from the Zircaloy cladding, including an IRF from the cladding, is assumed to be in organic form. The overall IRF thus contains a mixture of inorganic and organic ^{14}C.
- For Zircaloy cladding, a 20 % IRF of ^{14}C is assumed. Other radionuclides in the cladding are released congruently with cladding corrosion, which is assumed to occur at a constant rate.

Vitrified high-level waste:

- Vitrified HLW is solidified in thin stainless steel fabrication flasks, which are then placed in massive carbon steel canisters. The flasks are assigned no barrier function.
- During cooling of the glass, cracks form so that the surface area at the time of emplacement is greater than that of the original glass blocks.
- Following canister breaching, radionuclides in vitrified HLW are released congruently with glass dissolution at a constant rate per unit surface area of the waste.
- Glass fragments are conceptualised as a number of equal sized spheres, with a total volume equal to the total volume of glass, and a total surface area that accounts for the cracking of the glass. The surface area of the spheres decreases with time as they dissolve.

SF / HLW canister:

- All SF and HLW canisters are assumed to be breached simultaneously at a reference time of 10 000 years following waste emplacement. No initially defective canisters are present.
- The SF and HLW canisters are conservatively assumed to provide no physical barrier to water ingress or radionuclide release after they are breached.
- No credit is taken for the integrity of the SF Zircaloy cladding and the HLW fabrication flasks (i.e. breaching of the cladding and the fabrication flasks is assumed to occur immediately after canister failure).

Bentonite buffer:

- Radionuclides are assumed to be released to a well-mixed volume of water that corresponds to the void space within the canisters and is in contact with the inner boundary of the bentonite.
- The bentonite is assumed to be homogeneous in its transport properties in space and time. In particular, the thermally altered zone in the bentonite around the waste packages is assumed to be of negligible extent and any radiolytic oxidants formed near the wastes are assumed not to migrate significantly into the bentonite buffer.

- Reducing conditions are assumed to prevail within and around the repository. Solubility limits shared between isotopes of the same element and appropriate to reducing conditions constrain aqueous radionuclide concentrations. A radionuclide precipitates if the concentration of the corresponding element, summed over all isotopes, exceeds the solubility limit, and redissolution occurs if concentrations fall.
- The element concentrations used to evaluate whether solubility limits are exceeded are obtained by summing the concentrations of all isotopes originating from the waste. The background concentrations of isotopes originating elsewhere are conservatively ignored.
- In the case of radium, since the necessary data are available and because of the potential significance to safety of ^{226}Ra due to the very long half life of its parent ^{238}U, co-precipitation of radium with inactive isotopes of chemically similar elements is taken into account. For all other elements, however, immobilisation by co-precipitation is neglected, as is sorption of radionuclides on the corrosion products of the canisters and waste forms.
- The transport mechanism for solutes in the bentonite buffer is aqueous diffusion, described by Fick's law and retarded by linear, reversible, equilibrium sorption, described by an element-dependent sorption coefficient.
- Some radionuclides are subject to anion exclusion which affects their diffusion coefficients and the effective porosity they can access.
- Transport of radionuclides dissolved in water mediated by gas and/or tunnel convergence is considered to be negligible.
- Any radionuclide-bearing colloids are assumed to be immobile in the bentonite and are not considered.
- The axial diffusion of radionuclides into the bentonite buffer separating the canisters is conservatively neglected.

Long-lived intermediate-level waste:

- For ILW, release of radionuclides is assumed not to begin until a reference time of 100 years after waste emplacement due to incomplete resaturation at earlier times and due to immobilisation in the waste form.
- For times beyond 100 years, immobilisation of radionuclides in the waste form (e.g. activation products in hulls and ends from reprocessing) is conservatively neglected.
- By the time release begins, radionuclides in ILW are assumed to have migrated to the surrounding cementitious backfill, where they are uniformly mixed with porewater and partitioned between aqueous, sorbed and precipitated phases.
- Linear, equilibrium sorption is assumed, described by an element-dependent sorption coefficient (K_d).
- Solubility limits constrain radionuclide concentrations, with precipitation occurring if the solubility limits of the corresponding element, summed over all isotopes, are exceeded, and redissolution occurring, if concentrations fall.
- Radionuclide transport mediated by gas and/or tunnel convergence is considered to be negligible.

Host rock and confining units:

- The host rock consists of the "Opalinus Clay". The transport barriers provided by the confining units and the regional aquifers are conservatively neglected.
- The host rock is assumed to be homogeneous in its transport properties in space and time, with no discontinuities with significant transmissivities.
- Radionuclides are transported by diffusion described by Fick's law, and (very slow) advection described by Darcy's law.
- Both transport processes are retarded by retarded by linear, reversible, equilibrium sorption, described by an element-dependent sorption coefficient.
- Some radionuclides are subject to anion exclusion which affects their diffusion coefficients and the effective porosity they can access.
- Advection is driven by the currently observed pressure difference between lower and upper confining units. Glacial cycling and the currently observed overpressures within the host rock are assumed to have negligible effects on advective transport.
- The impact of gas on transport is assumed to be insignificant.
- Colloids are assumed to have no impact on radionuclide transport, on account of the fine pore structure of the host rock.
- Uplift and erosion are assumed to have negligible effects on the hydraulic properties of the host rock over the time period of interest.
- It is assumed that no radionuclides are transported along tunnels, ramps and shafts.
- Radionuclides that are released from upper and lower boundaries of the Opalinus Clay are assumed to be transferred instantaneously to the biosphere.
- Transport times through the sedimentary layers overlying and underlying the host rock, including the confining units that in reality are expected to contribute significantly to retention, are conservatively neglected.
- Dilution in deep regional aquifers is small compared to that assumed to occur in shallow aquifers and in the surface environment, and is neglected.

4.2.2 Input parameters and probabilistic analyses

The relevant data from Project Opalinus Clay which form the basis of the probabilistic analyses have been reproduced from Nagra (2002a and b) in Appendix B. In order to investigate the sensitivity of calculated doses to model chain input parameters in a comprehensive manner, those parameters that are known to influence the release and transport of radionuclides substantially are sampled stochastically. Among them are (*cf.* Nagra 2002b):

- Parameters controlling the release of radionuclides from SF: Cladding dissolution rate, instant release fraction IRF, SF matrix dissolution rate.
- Parameter controlling the release of radionuclides from virtrified HLW: glass dissolution rate.
- Parameters controlling the transport behaviour of radionuclides in the SF/HLW (bentonite) and ILW (cement) near field: Radionuclide solubilities, sorption coefficients and effective diffusion coefficients (only bentonite).

- Parameters controlling the transport behaviour of radionuclides in the geosphere: Transport path length in Opalinus Clay, effective diffusion coefficients in Opalinus Clay, sorption coefficients in Opalinus Clay, Darcy velocity in Opalinus Clay.

In the analyses, the probabilistic parameters for individual model runs are selected from probability density functions (PDFs). These PDFs take one of a number of standard forms:

- uniform
- log-uniform
- triangular
- log-triangular
- discrete
- normal
- log-normal

The first five lie between optimistic and pessimistic bounding values, while normal and log-normal PDFs are generally unbounded. However, upper and / or lower cut-off values can be chosen, beyond which a normal or log-normal PDF is truncated and assumed to take a zero probability.

The PDFs of the probabilistic parameters are listed in Tab. B-16 along with additional parameter values and references to other data tables in Appendix B.

4.2.3 Integration of tools and application

The conceptualisation of the key phenomena described above forms the basis of a set of governing equations, with accompanying initial conditions and boundary conditions, that are solved using the computer codes STMAN for the near field and PICNIC for the host rock, together with biosphere dose conversion factors (BDCFs) for the surface environment. The reference model chain STMAN-PICNIC is used to model the radionuclide release and migration of a range of radionuclides that are judged to be safety relevant, and the doses to which these give rise. The selection of safety-relevant radionuclides is discussed in Nagra (2002b).

Using GoldSim, 1000 sets of samples with probabilistically determined parameter values are generated each for SF, vitrified HLW and ILW. Via the DLL-interface and specific Python scripts, these samples are processed further to finally obtain input data files – including the deterministic model parameters – to be used by STMAN and PICNIC. The calculated radionuclide fluxes out of the host rock are multiplied by the BDCFs to quantify the radiological consequences. Finally, the resulting dose values are evaluated using the statistical functionality of GoldSim.

4.2.4 Results

The temporal evolution of the median dose, the 95^{th} and 5^{th} percentiles and the highest and lowest dose maxima of all realisations for SF, HLW and ILW, each based on a set of 1000 calculations, is shown in Fig. 4.2-2. Generally, the band width between the highest and the lowest maximum is three or more orders of magnitude. The highest maximum dose value of 4.3×10^{-4} mSv/a results for SF, the lowest maximum dose value for HLW (4×10^{-12} mSv/a).

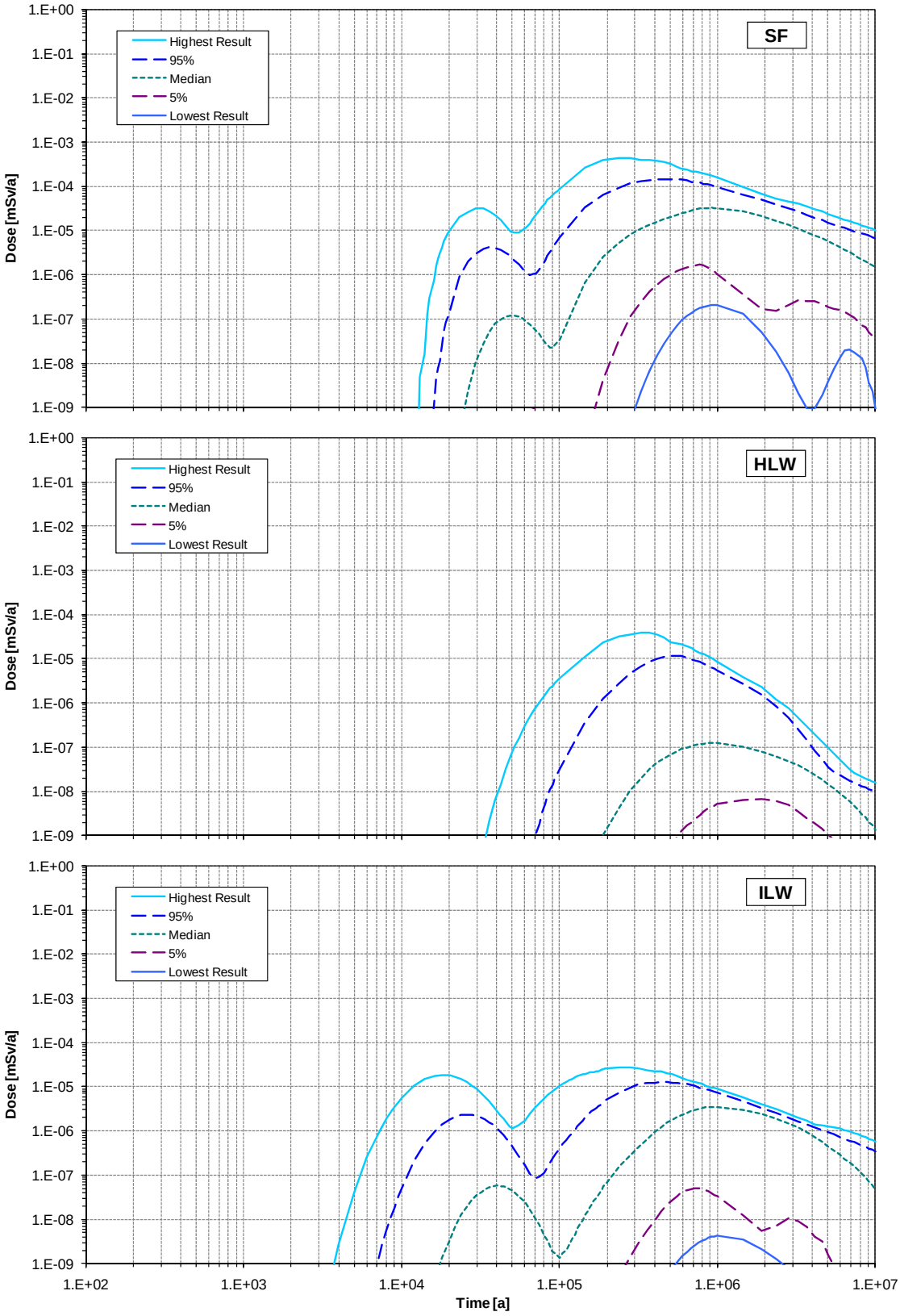


Fig. 4.2-2: Evolution of the median, the 95th percentile, the 5th percentile and the highest and lowest results of all samples for SF, HLW and ILW.

Fig. 4.2-2 may be compared with Fig. 7.4-3b from Project Opalinus Clay (Nagra 2002a), which was calculated using the same near field and geosphere transport codes, but a different, purpose-built probabilistic driver (GIPC, see Nagra 2002b). The agreement is excellent.

The complementary cumulative distribution functions CCDF for SF, HLW and ILW are shown in Fig. 4.2-3. The 50 % percentile, i.e. the maximum dose value that is exceeded by 50 % of all samples, is 3.67×10^{-5} mSv/a for SF, 1.27×10^{-7} mSv/a for HLW and 3.68×10^{-6} mSv/a for ILW.

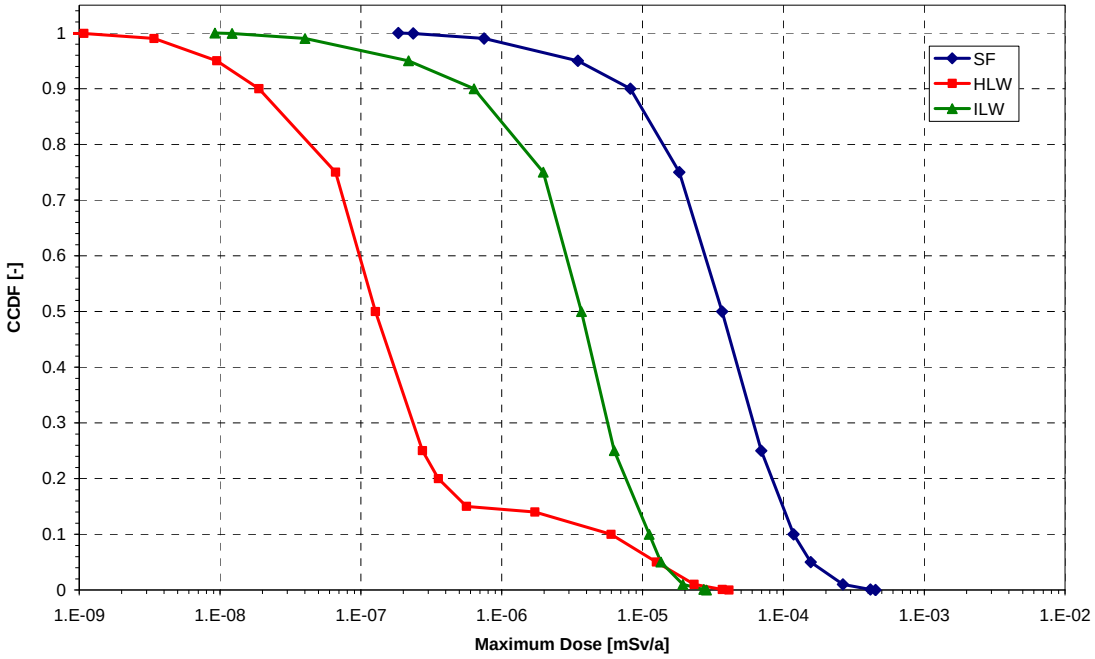


Fig. 4.2-3: Complementary Cumulative Distribution Function CCDF for SF, HLW and ILW.

Fig. 4.2-3 may be compared with Fig. 7.4-3a from Project Opalinus Clay (Nagra 2002a). Again, the agreement is excellent.

To assure the quality of probabilistic analyses, the number of realisations must be sufficiently large to obtain accurate results and make statistically reliable predictions. Fig. 4.2-4 exemplifies this aspect for the model runs for SF. It shows the maximum dose value for each of the 1000 realisations, and the resulting moving average[5]. This moving average stabilises after approximately 150 realisations. The same applies for the calculations considering HLW and ILW. Together, this result clearly indicates that 1000 realisations are adequate for a reliable interpretation.

[5] The "moving average" for realisation *n* is defined as (1/n) $\sum D_{max}(i)$, where $D_{max}(i)$ is the maximum dose of realisation *i* and the index *i* runs from 1 to *n*.

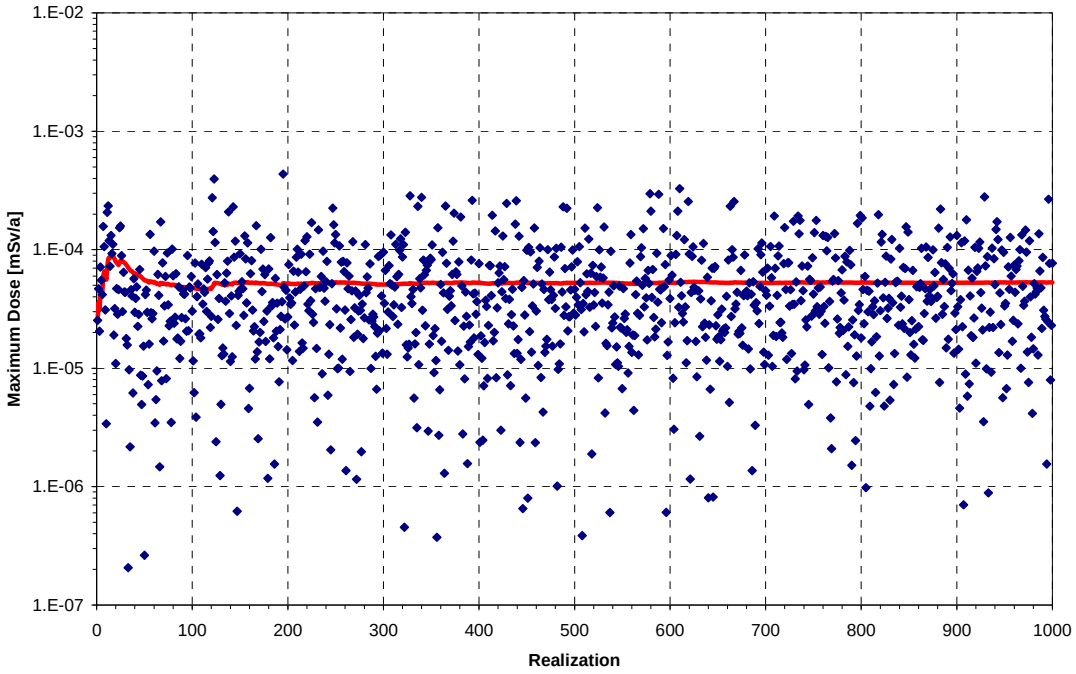


Fig. 4.2-4: Maximum dose of each realisation and moving average (red curve, mean) over the number of realisations for SF.

Another import analysis of probabilistic calculations is the determination of possible correlations between model parameters and the modelled results, i.e. the maximum dose values. For the high-level wastes, these correlations are generally rather weak. Only very few parameters significantly influence the resulting maximum dose (Fig. 4.2-5). For SF, where the dose maxima are in most cases dominated by the release of ^{129}I, these parameters are:

- the Darcy velocity in Opalinus Clay,
- the Instant Release Fraction IRF of iodine in the waste,
- the sorption coefficient of iodine in Opalinus Clay,
- the effective diffusion coefficients in Opalinus Clay, and
- the length of the geosphere transport path in Opalinus Clay.

In case of HLW, the dose maxima result from ^{79}Se, and the model parameters correlated to these maxima are:

- the solubility limit of selenium in the bentonite near field,
- the Darcy velocity in Opalinus Clay,
- the length of the geosphere transport path in Opalinus Clay, and
- effective diffusion coefficients in Opalinus Clay.

Considering ILW, the dose maxima are again mostly dominated by ^{129}I. The model parameters correlated to the dose maxima are:

- the Darcy velocity in Opalinus Clay,
- the sorption coefficient of iodine in Opalinus Clay,

- the effective diffusion coefficients in Opalinus Clay, and
- the length of the geosphere transport path in Opalinus Clay.

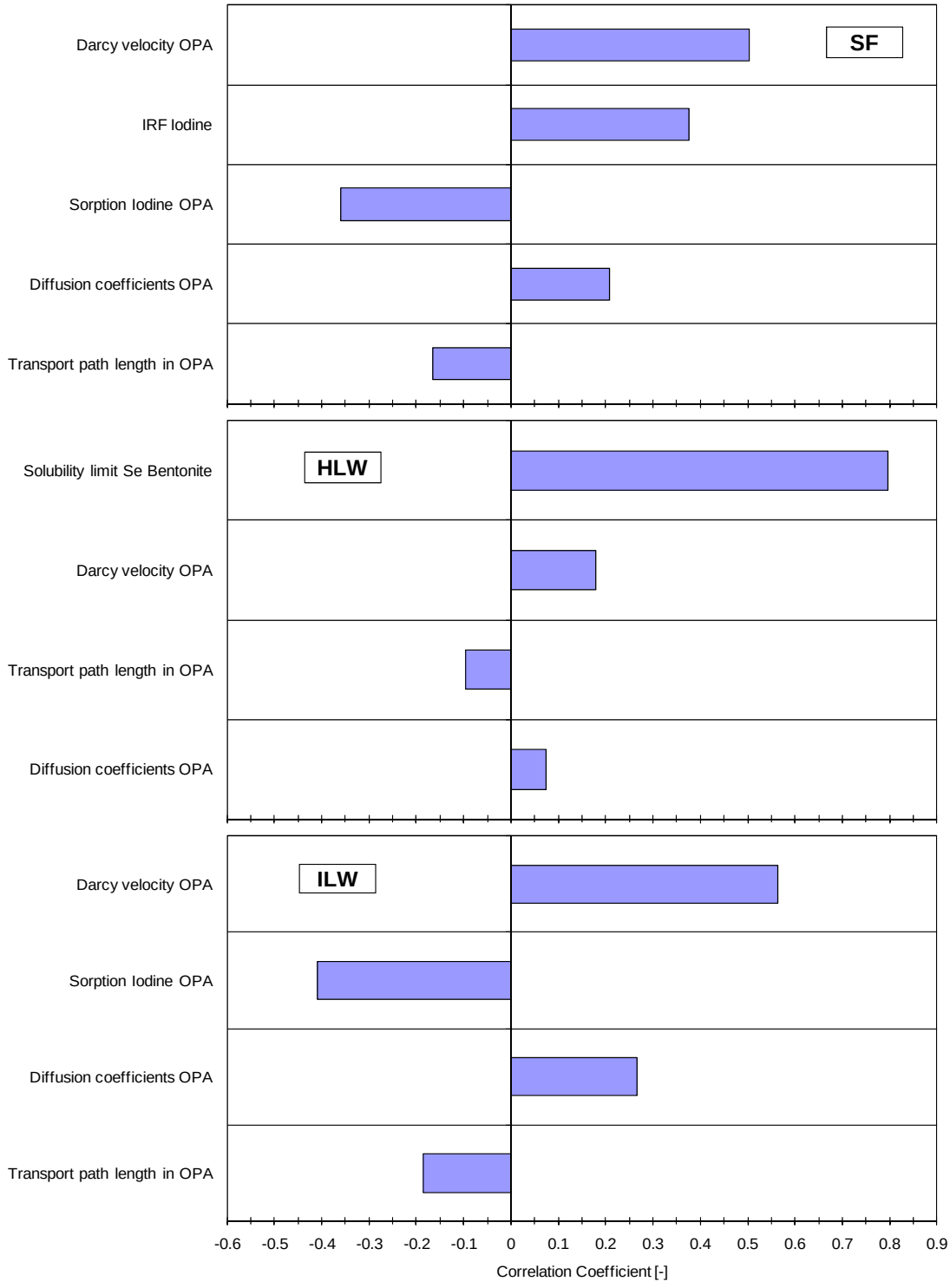


Fig. 4.2-5: Parameter correlation with maximum peak dose for SF, HLW and ILW.

The temporal evolution of the mean dose for SF, HLW and ILW, each based on a set of 1000 calculations, is shown in Fig. 4.2-6. The sum dose is dominated by the contribution from SF. Only at early times up to about 20'000 years, the ILW defines the sum dose.

For all types of high- and intermediate-level wastes, the non-sorbing or weakly sorbing fission and activation products ^{129}I, ^{36}Cl, organic ^{14}C and ^{79}Se define the sum dose (Fig. 4.2-7). Regarding all other radionuclides that are released from the different waste forms, no significant flux into the biosphere can be observed within 10 million years. These results emphasise the very good barrier efficiency of the Opalinus Clay host rock formation.

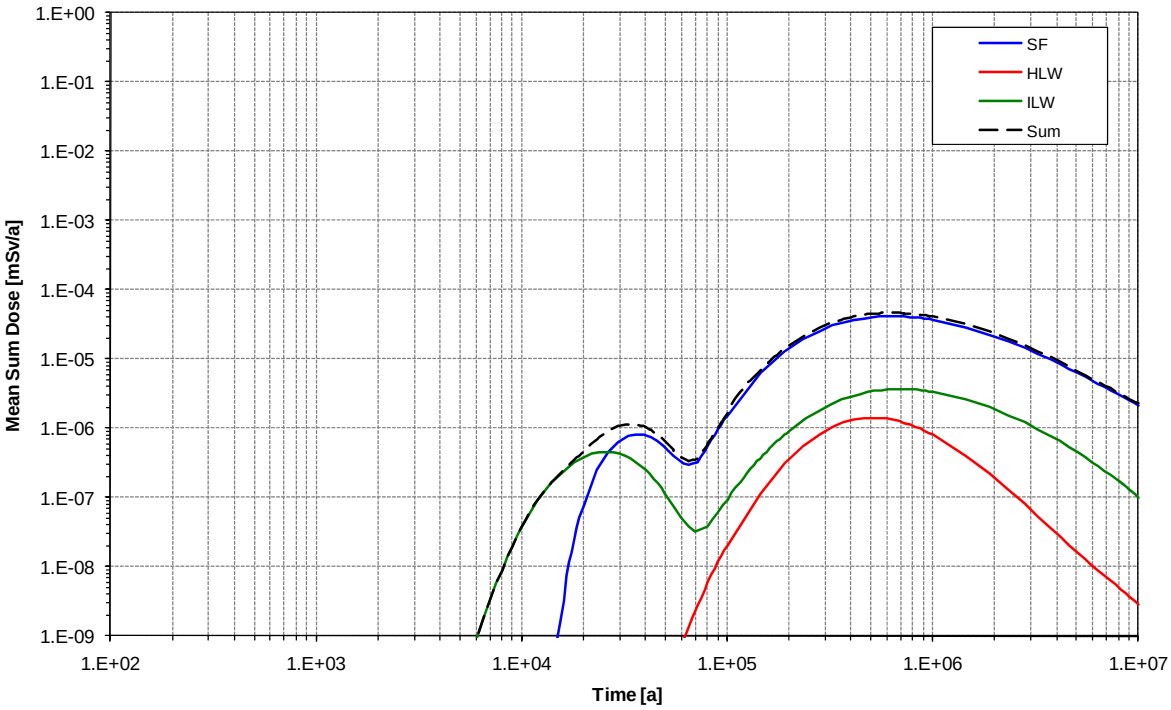


Fig. 4.2-6: Mean sum dose as a function of time, for SF, HLW and ILW.

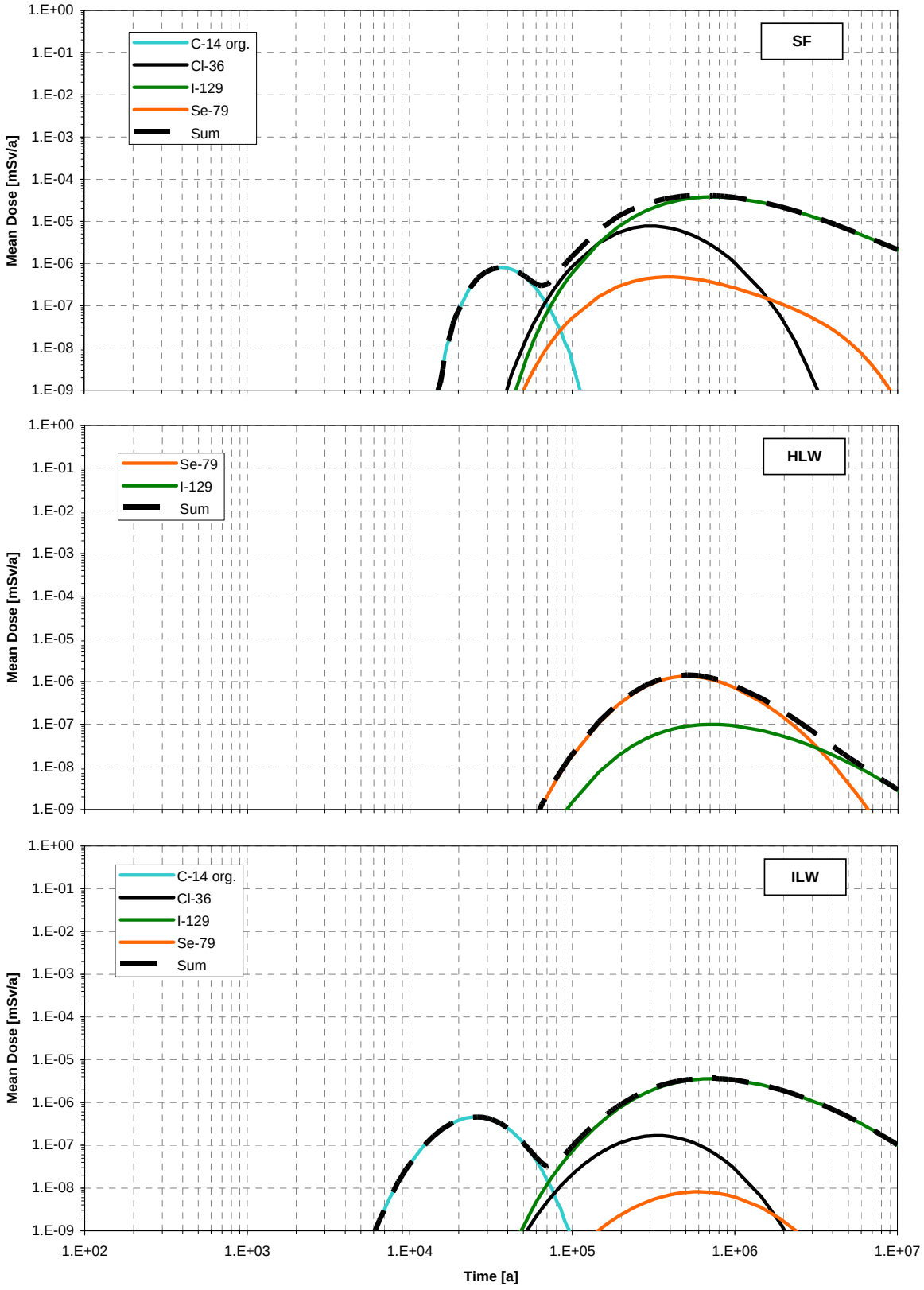


Fig. 4.2-7: Mean dose as a function of time for SF, HLW and ILW.

4.3 Application for a repository for L/ILW

4.3.1 Conceptual model and data

In this study, the general conceptualisation is based on a generic L/ILW repository as defined in the safety report (Nagra 2008a) compiled for stage 1 of the Sectoral Plan for Deep Geological Repositories (SFOE 2008).

The conceptual model for a generic repository for L/ILW is based on a number of assumptions regarding the conceptualisation for modelling purposes of key FEPs associated with the various system components that comprises some pessimistic or conservative conceptual assumptions and parameter values. Considering the near field and the waste forms, these are the following:

- In the case of L/ILW, the waste forms, emplacement containers and the backfilled cementitious mortar are assumed to be homogeneously mixed.
- The release of radionuclides is assumed to begin immediately with the post-closure phase. The radionuclides are assumed to be instantaneously and uniformly mixed within the porewater of the waste / cementitious mortar and partitioned between aqueous and sorbed phases.
- Linear, reversible, equilibrium sorption is assumed, described by an element-dependent sorption coefficient. Due to the flow-induced porewater exchange in the caverns, the cement is assumed to be degrading, resulting in a deterioration of the sorption behaviour of the radionuclides. The transition between a fresh, non-degraded cemetitious near field and degraded near field is linear in time and depends on the water flow rate in the host rock and in the cavern, respectively.
- Transport of radionuclides dissolved in water driven by gas and/or tunnel convergence is considered to be negligible.

The conceptual assumptions regarding the host rock, the confining units and the biosphere are the same as for HLW described in Chapter 4.2.1. L/ILW-specific model parameters are given in Appendix C.

4.3.2 Input parameters and probabilistic analyses

The relevant data from Project Opalinus Clay which form the basis of the probabilistic analyses have been reproduced from Nagra (2002a and b) in Appendix B. The stochastically generated parameters of the probabilistic calculations for L/ILW are those that most strongly influence the release and transport of radionuclides. These are:

- Parameters controlling the transport behaviour of radionuclides in the cementitious near field: Radionuclide sorption coefficients and their temporal evolution (timescale of degradation)
- Parameters controlling the transport behaviour of radionuclides in the geosphere: Transport path length in Opalinus Clay, effective diffusion coefficients in Opalinus Clay, sorption coefficients in Opalinus Clay, Darcy velocity in Opalinus Clay

In the analyses, the probabilistic parameters for individual model runs are selected from probability density functions (PDFs). The PDFs of the probabilistic parameters for L/ILW are listed in Tab. C-5 along with additional parameter values and references to other data tables in Appendix B and Appendix C.

4.3.3 Integration of tools and application

Following the given conceptualisation, the release and transport of a set of safety relevant radionuclides is calculated using the computer codes VPAC for the near field and PICNIC for the host rock. The selection of safety-relevant radionuclides for L/ILW is given in Nagra (2008a). Biosphere dose conversion factors (BDCFs) are used for a simplified representation of the influence of the surface environment and to calculating the doses to which the radionuclide release gives rise.

In terms of a generic L/ILW repository, caverns with a length of 195 m each and a horizontal distance of 85 m are considered (Nagra 2005). A thickness of 300 m for the host rock section is considered (150 m below and 150 m above the mid plane of the cavern). The water flow in the host rock is assumed to be vertically upward[6]. The model geometry (FE grid) for the case of a homogeneous porous host rock is shown in Fig. 4.3-1. Because of the symmetry only one half of the cavern and the adjacent host rock up to the mirror plane between to caverns is modelled with VPAC. Parallel to the main axis of the cavern (z direction) an arbitrary length of 1 m is assumed.

The inner part of the cavern is modelled as one homogeneous material consisting of the waste packages, the containers and the cementitious mortar backfill. This material class is called "backfill". The cavern liner has the same properties but without an initial radionuclide inventory (material class "cavern liner").

The retardation of radionuclides by sorption in the near field depends on the cement content (undegraded) and on the calcite fraction (degraded). Their change with time is caused by exchange of pore solution in the near field. Thus, a variable sorption is modelled in VPAC by time-dependent K_d values. In a first phase the K_d values are those for fresh cement (typically "good" sorption). This phase is followed by a second phase with a linear decrease of cement content and increase of calcite fraction and the corresponding linear change of K_d values. In a third phase sorption values for degraded cement (typically poorer sorption) are assumed. The duration of the individual phases depends on the exchange of pore solution in the cavern, that itself depends on the water flow through the cavern (Nagra 2008d). Solubility limits are conservatively neglected for the near field.

The ^{14}C inventory is classified waste specifically into the three fractions "inorganic", "organic with instant release" and "organic with congruent release". For the congruent release it is assumed that it is constrained by the corrosion of the waste matrix. Based on pessimistic assumptions for corrosion rates and geometry a simplified constant fractional release rate of 10^{-4} per year is assumed (Nagra 2008d).

The radionuclide release rate calculated with VPAC serves as input for calculating the radionuclide transport within the geosphere with the PICNIC code. Unfractured host rock is modelled as a homogeneous porous medium within a single one-dimensional PICNIC leg. The retardation of radionuclides by sorption in the geosphere is modelled by element-specific K_d values. Solubility limits are conservatively neglected for the geosphere.

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[6] The influence of different flow directions to the cavern on the radionuclide release has been investigated. It could be shown that the release rates for the most important radionuclides and a broad spectrum of hydrogeological situations are only slightly dependent on the flow direction (Nagra 2008c). Because of symmetry effects in case of a vertical flow direction the FE grid is much smaller than in case of horizontal flow. Thus, for this study generally horizontal flow was considered.

Using GoldSim, 1000 sets of samples with probabilistically determined parameter values are generated for L/ILW. Via the DLL-interface and specific Python scripts, these samples are processed further to finally obtain input data files – including all deterministic model parameters – to be used by VPAC and PICNIC. The calculated radionuclide fluxes from the host rock are multiplied by the BDCFs to quantify the radiological consequences. Finally, the resulting dose values are evaluated using the statistical functionality of GoldSim.

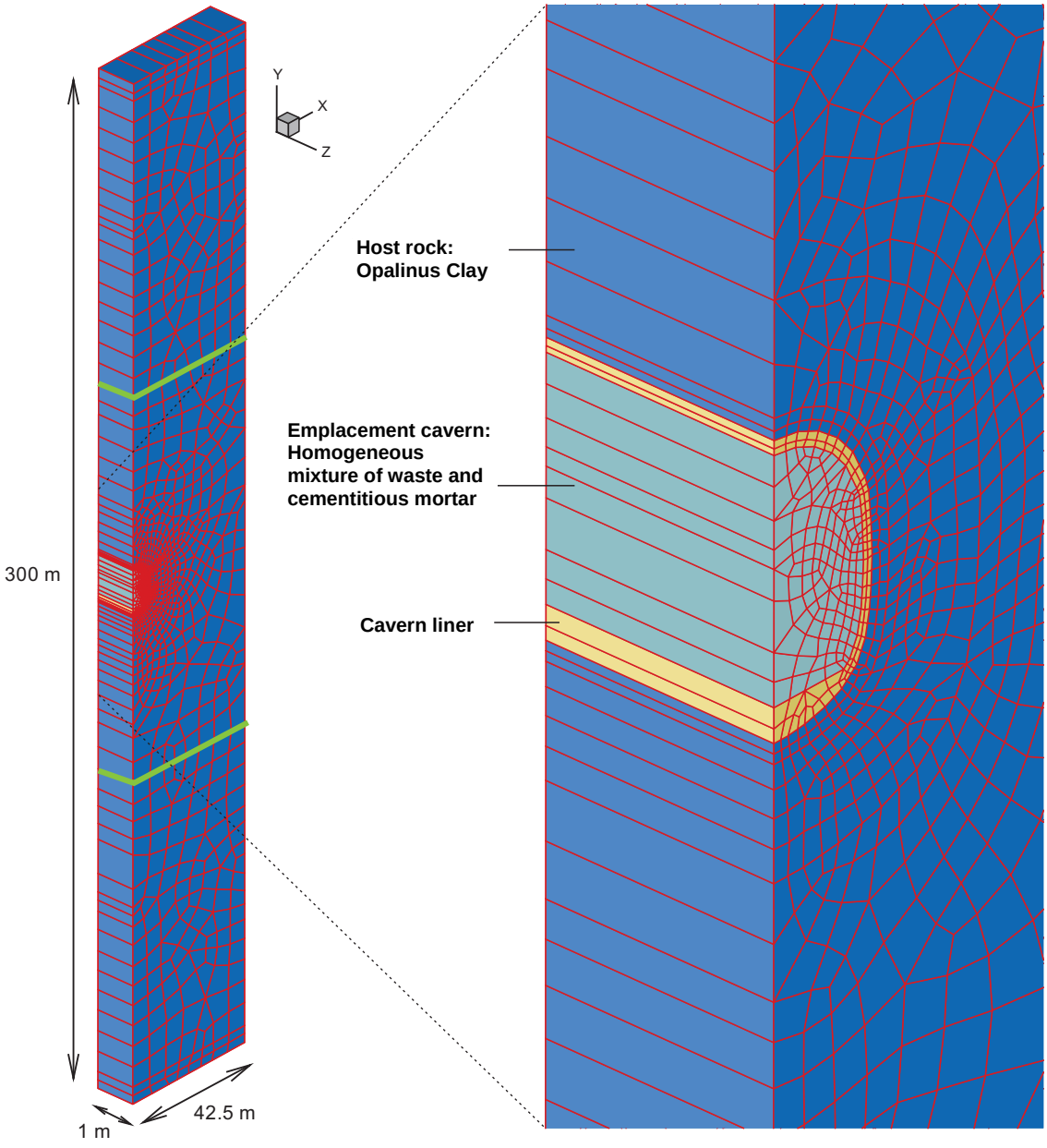

Fig. 4.3-1: Model geometry in VPAC for L/ILW in case of a homogeneous porous host rock without fractures.

4.3.4 Results

The temporal evolution of the median dose, the 95th and 5th percentiles and the highest and lowest dose maxima of all realisations for L/ILW, based on a set of 1000 calculations, is shown in Fig. 4.3-2. Generally, the band width between the highest and the lowest maximum is more than four orders of magnitude. The highest maximum dose value is 2×10^{-2} mSv/a, the lowest maximum dose value 1.2×10^{-6} mSv/a. The highest maximum dose values occur between a few hundred and approximately 50'000 years.

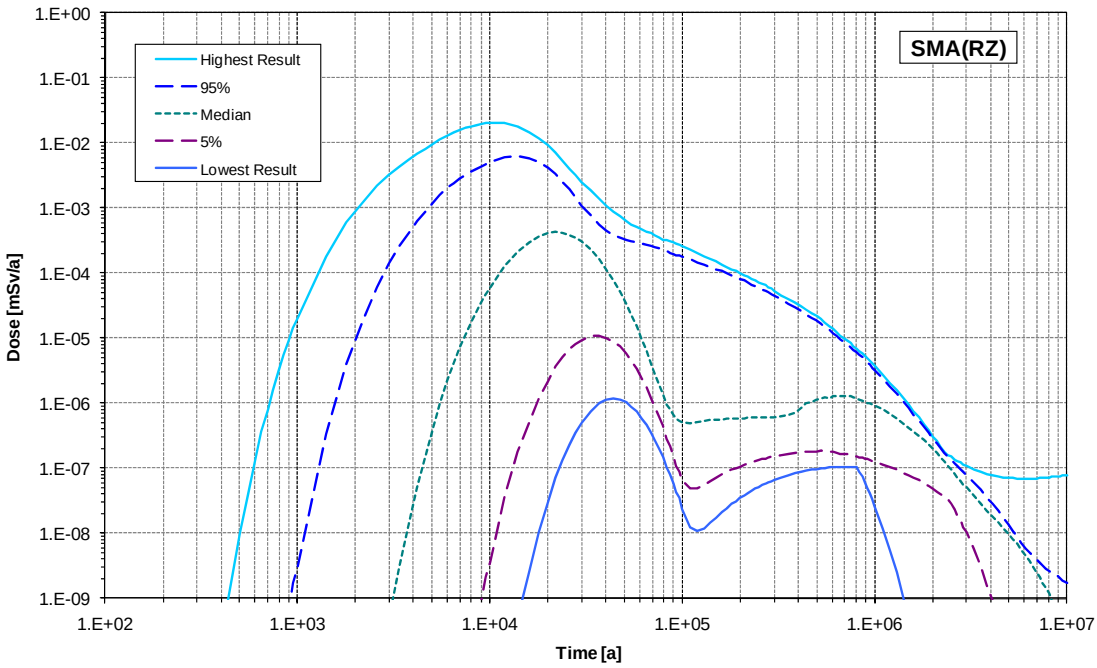

Fig. 4.3-2: Evolution of the median, the 95th percentile, the 5th percentile and the highest and lowest results of all samples for L/ILW.

The complementary cumulative distribution function CCDF for L/ILW is shown in Fig. 4.3-3. The 50 % percentile, i.e. the maximum dose value that is exceeded by 50 % of all samples, is 4.25×10^{-4} mSv/a.

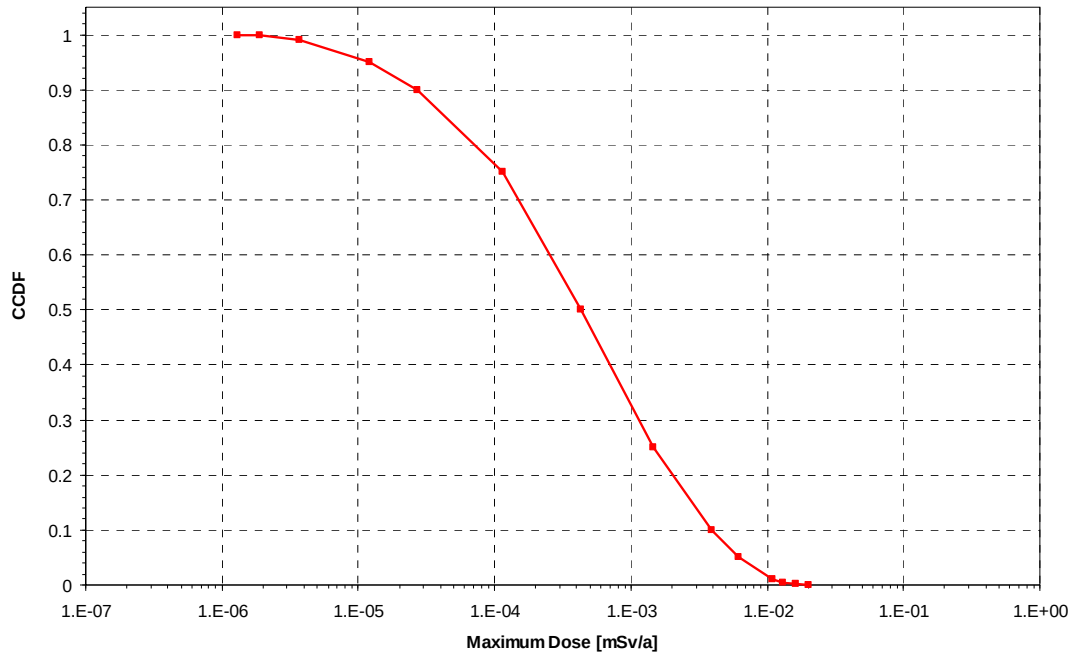

Fig. 4.3-3: Complementary Cumulative Distribution Function CCDF for L/ILW.

Fig. 4.3-4 shows the maximum dose value for each of the 1000 realisations, and the resulting moving average. This moving average stabilises after approximately 300 realisations.

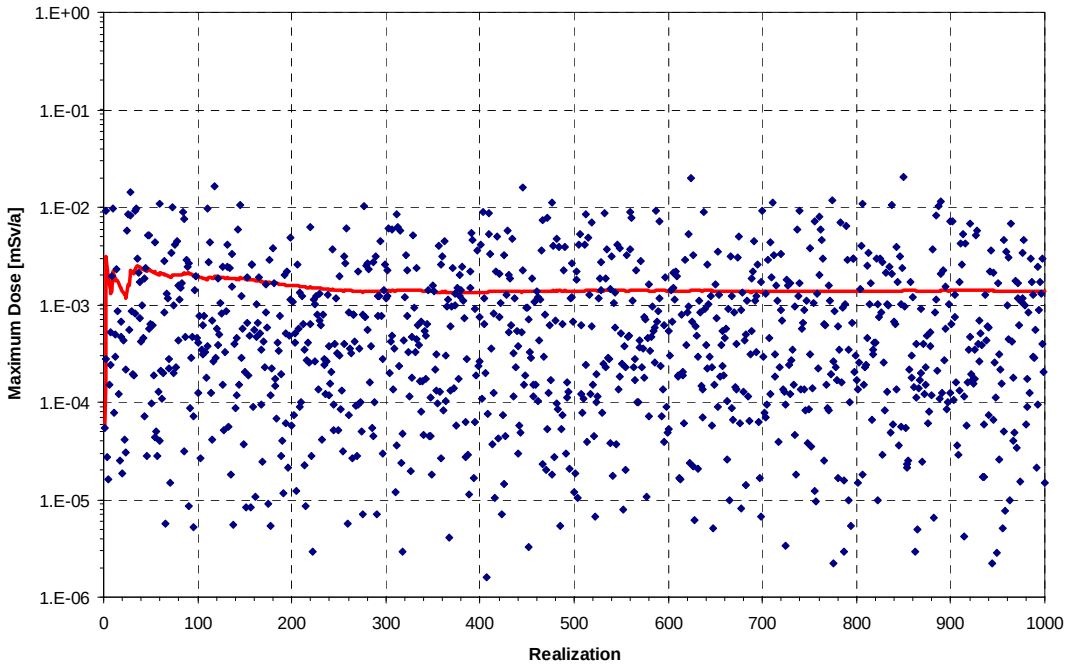

Fig. 4.3-4: Maximum dose of each realisation and moving average (red curve, mean) over the number of realisations for L/ILW.

As for the high-level wastes, the correlations between the probabilistic model parameters and the modelled results, i.e. the maximum dose values, are relatively weak. Only three parameters exhibit a significant influence on the resulting maximum dose (Fig. 4.3-5). These parameters are:

- the length of the geosphere transport path in Opalinus Clay,
- the effective diffusion coefficients in Opalinus Clay, and
- the Darcy velocity in Opalinus Clay.

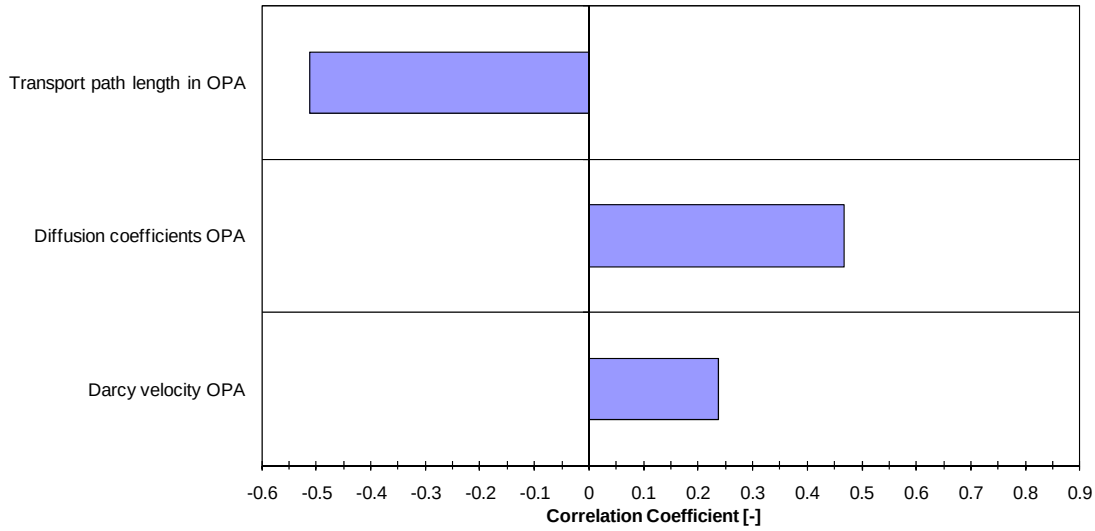

Fig. 4.3-5: Parameter correlation with maximum peak dose for L/ILW.

The temporal evolution of the mean dose for L/ILW, based on a set of 1000 calculations, is shown in Fig. 4.3-6. The non-sorbing or weakly sorbing fission and activation products ^{108M}Ag, organic ^{14}C (instant and congruent release), ^{36}Cl, ^{79}Se, ^{129}I and ^{40}K define the sum dose. Regarding all other radionuclides that are released from the waste, no significant flux from the host rock can be observed at any time.

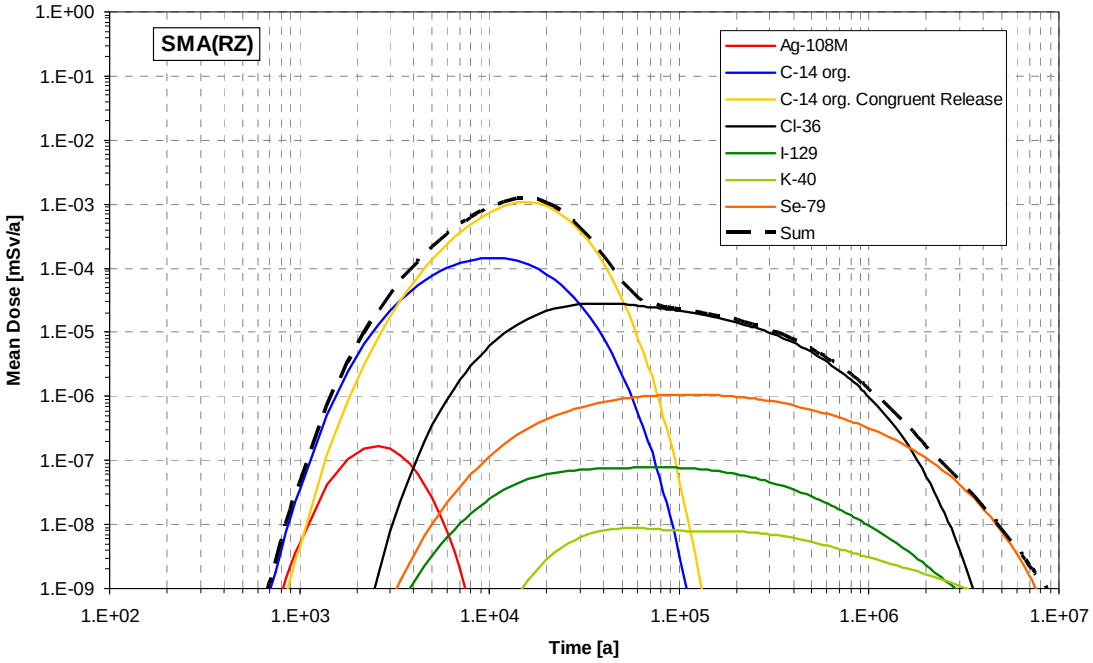

Fig. 4.3-6: Mean dose as a function of time for L/ILW.

5 Simplified PSA modelling using GoldSim RT

This chapter describes an alternative, independently performed simplified probabilistic safety assessment using the data from the Swiss Opalinus Clay project (Nagra 2002a) and the radionuclide transport module of the GoldSim code (hereafter called GoldSim RT). This work was conducted by ENRESA complementarily to the calculations done by AF-Colenco for the same disposal concept (see Chapter 4 above). The remainder of this chapter contains the material presented in the independent milestone report by ENRESA (2009).

5.1 Models

The repository concept and the models are described in Nagra (2002a and b). The input probability distribution functions for probabilistically sampled parameters can be found in Nagra (2006). A 2D GoldSim RT model was developed for each of the 5 different wastes: SF, HLW reprocessed by COGEMA (France), HLW reprocessed by BNFL (UK), ILW *without* significant concentrations of low molecular weight organics and other complexing agents (waste group ILW-1) and ILW *with* significant concentrations of low molecular weight organics and other complexing agents (waste group ILW-2). Each model represents the length of disposal tunnel and the fraction of host formation that correspond to a single waste package.

GoldSim RT uses a mixing cell algorithm for the transport in porous media that involves the discretisation of the medium into a number of mixing cells with the following characteristics:

- The mixing in the cell is complete and instantaneous.
- A cell may contain different media (water, bentonite, clay etc.).
- Radionuclides in a cell are distributed between the different media in the cell according to their distribution coefficients (K_d).
- Diffusive and advective solute transport between cells are modelled.

In the cells, the following processes are considered:

- Radioactive decay / ingrowth for decay chains with no limit to the number of members
- Precipitation (solubility limits) / redissolution
- Different isotopes of the same chemical element; and, as a consequence, elemental solubility is shared between the different isotopes of the element
- Anion exclusion (i.e. accessible porosity can be element specific).

Mass transfer between adjacent cells is considered to create advective and diffusive connections.

Fig. 5.1-1 presents the model developed for SF. Similar models are used for Cogema and BNFL HLW, with only small geometric differences. The models for ILW-1 and ILW-2 do not include bentonite but there is concrete in the circular (blue) cell where the radionuclides are released.

The model includes diffusion, anion exclusion and sorption in the host rock and bentonite. It also includes advection in the host formation due to the upwards directed groundwater flow. However, advection is not considered in the bentonite.

The boundary conditions in the model are:

- no flux through lateral surfaces, and
- zero concentration in the top and bottom of the host formation.

In addition to the 2D models, simplified 1D models were created for the five different wastes, using thirty "box" cells to represent the formation above the repository level and thirty "box" cells to represent the formation below repository level.

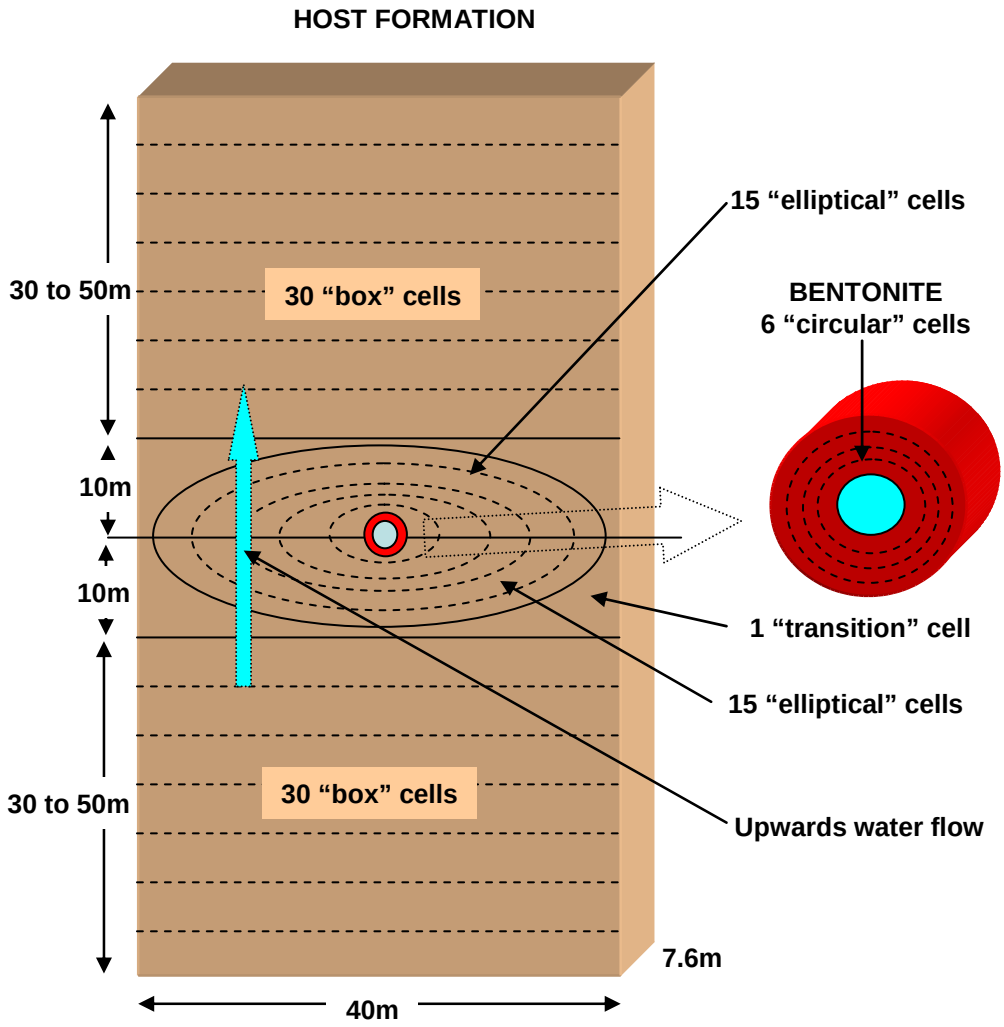

Fig. 5.1-1: GoldSim RT 2D model for SF.

5.2 Results from the 2D model runs

This section presents the results of the 1000-runs probabilistic calculation conducted by ENRESA using the 2D models. Fig. 5.2-1 is an overview of the mean doses for the 5 different wastes. The total dose is controlled by ILW-1 up until about 20'000 years and by SF thereafter.

Fig. 5.2-2 to Fig. 5.2-6 present the radionuclides that produce meaningful doses for each of the 5 different wastes. The doses from Cogema HLW and BNFL HLW are very similar. The doses for ILW-2 are much smaller than the doses for ILW-1.

Only non-sorbing or weakly sorbing fission and activation products cause doses above 10^{-12} mSv/a: ^{129}I, ^{36}Cl, organic ^{14}C, ^{79}Se and ^{41}Ca. No significant amounts of actinides or daughters are released from the host rock at any time because of the strong sorption on the host formation.

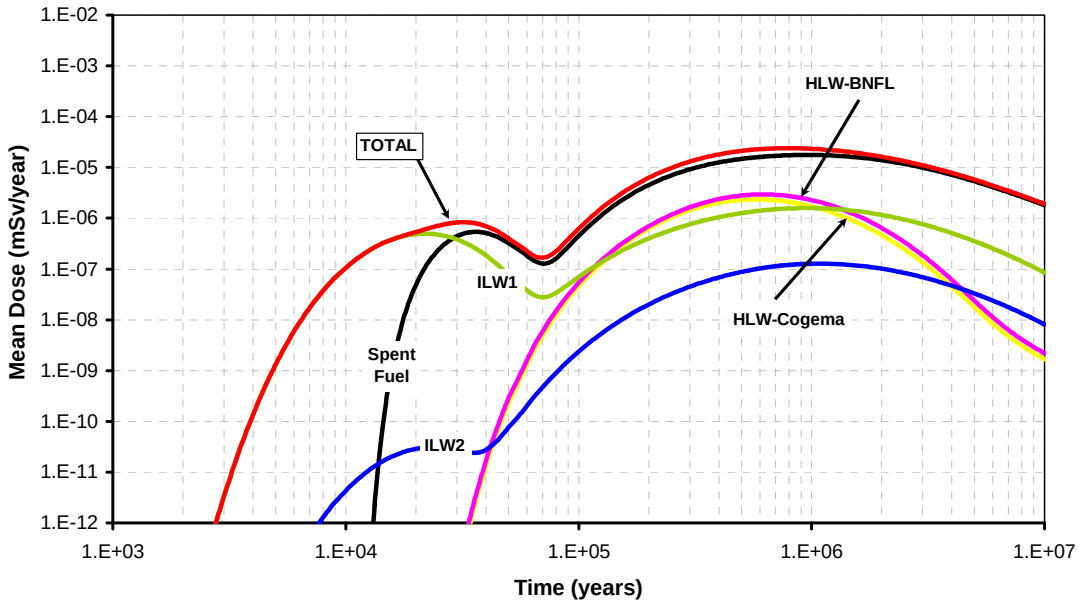

Fig. 5.2-1: Mean doses for the 5 different wastes, calculated with the 2D model.

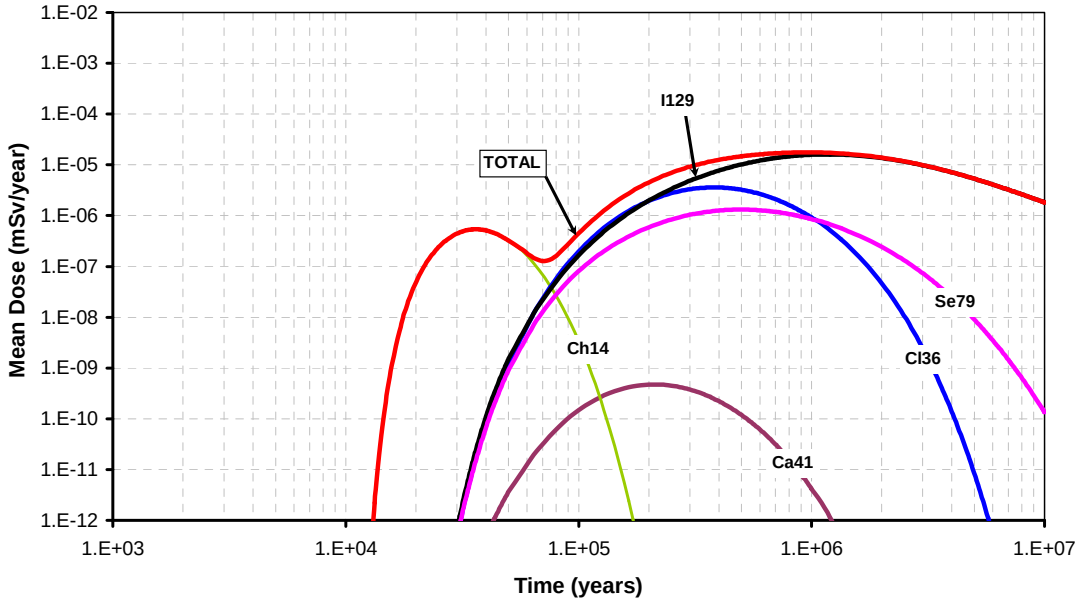

Fig. 5.2-2: Doses for SF: Mean dose per radionuclide and total.
"Ch14" is shorthand notation for "C-14 org.".

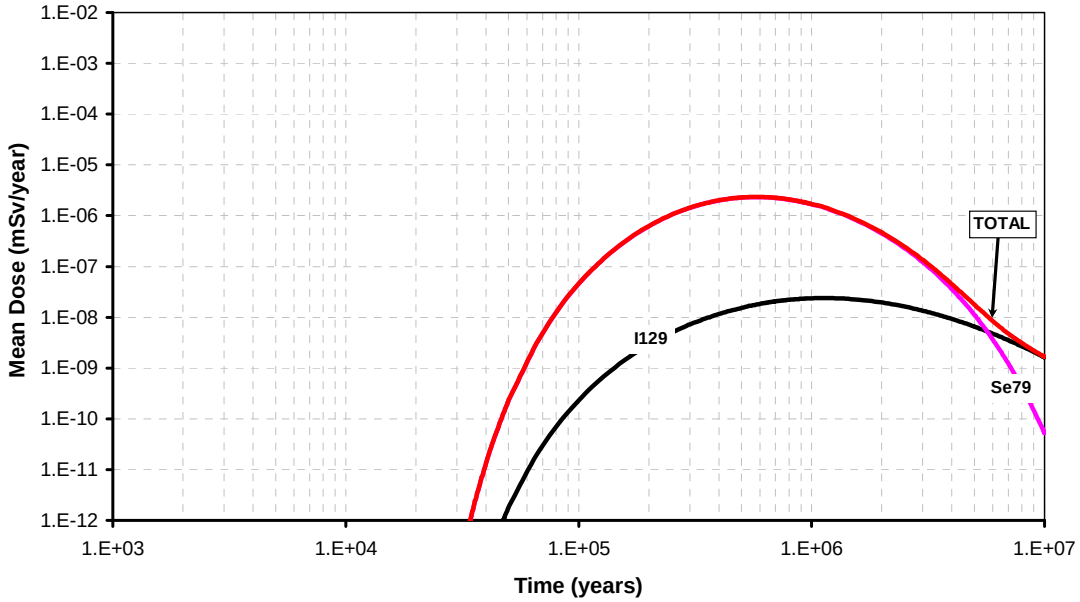

Fig. 5.2-3: Doses for Cogema HLW: Mean dose per radionuclide and total.

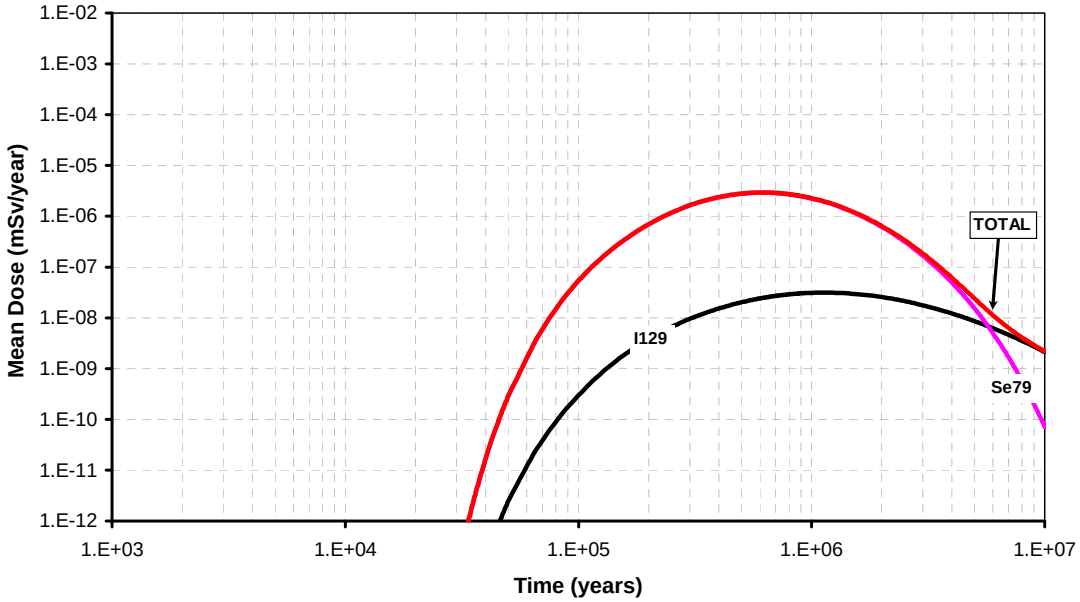

Fig. 5.2-4: Doses for BNFL HLW: Mean dose per radionuclide and total.

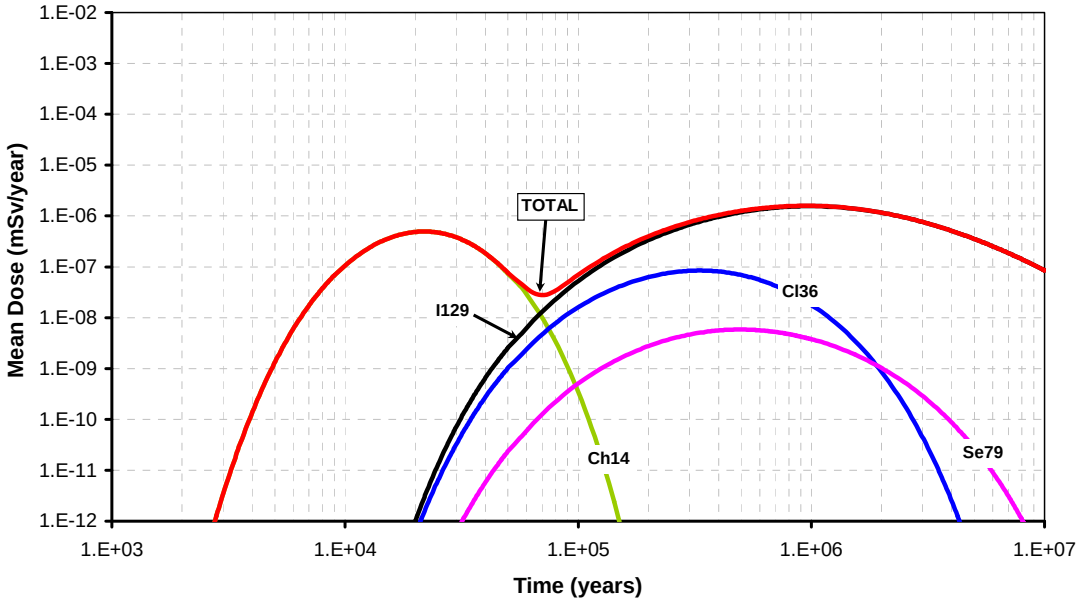

Fig. 5.2-5: Doses for ILW-1: Mean dose per radionuclide and total.
"Ch14" is shorthand notation for "C-14 org.".

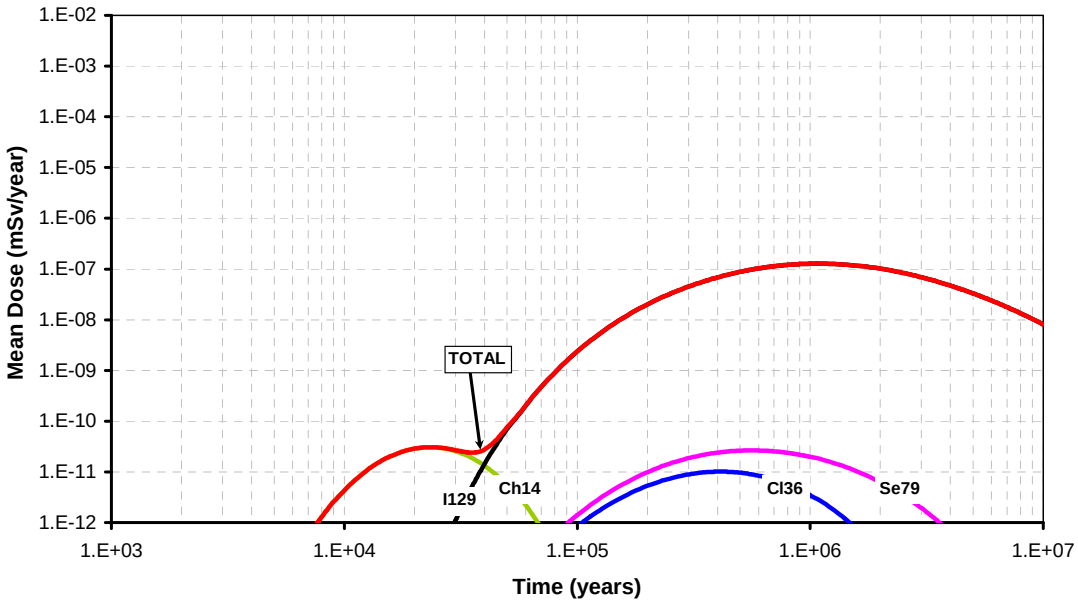

Fig. 5.2-6: Doses for ILW-2: Mean dose per radionuclide and total.
"Ch14" is shorthand notation for "C-14 org.".

5.3 Results from the 1D models

Fig. 5.3-1 presents the mean doses for the 5 different wastes as calculated using 1D models. The results are very similar to those from the more realistic 2D models (Fig. 5.2-1), and show that these 1D models can be considered as more "conservative", i.e. doses start earlier and peak doses are slightly higher.

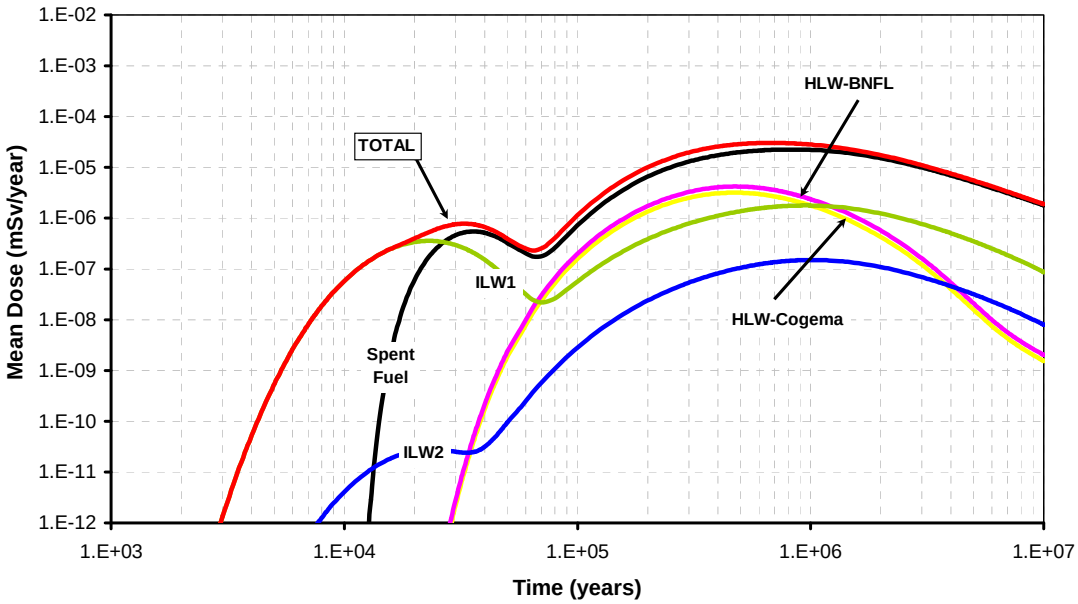

Fig. 5.3-1: Mean doses for the 5 different wastes, calculated with the 1D model.

6 Comparison of results from the two independently performed simplified PSA calculations using pre-existing Nagra codes and GoldSim RT

In Chapter 4, simplified PSA calculations using the GoldSim Monte-Carlo simulator to run the deterministic Nagra codes STMAN and PICNIC in a probabilistic mode were introduced. In Chapter 5, similar calculations employing both the GoldSim Monte-Carlo simulator and the radionuclide transport module of the GoldSim package, GoldSim RT, were presented. In the present chapter, the results from these two independently-performed sets of calculations are compared.

Fig. 6.4-1 shows the mean doses for SF, HLW and ILW as obtained by the two different modelling approaches. Tab. 6.4-1 summarises the dose maxima. The agreement between the results can generally be judged as reasonable, considering that the conceptualisation of the system is quite different in the two approaches, with the STMAN/PICNIC model chain consistently yielding higher dose values. Between the two modelling approaches the differences in maximum dose values are about a factor of 2 or less. Since the input parameters used in the two approaches were identical, this difference can be viewed as a measure of the influence of using alternative conceptualisations (1D vs. 2D, different conceptualisation of the interface between the near field and the host rock).

Regarding the correlations between the probabilistic model parameters and the modelled results, i.e. the maximum dose values, the agreement between the results of the STMAN/PICNIC calculations and the GoldSim RT calculations is relatively good (Fig. 5.4-2). Those parameters that effectively influence the maximum dose values are clearly identified by both approaches, although the order of these parameters differs between the two sets of results.

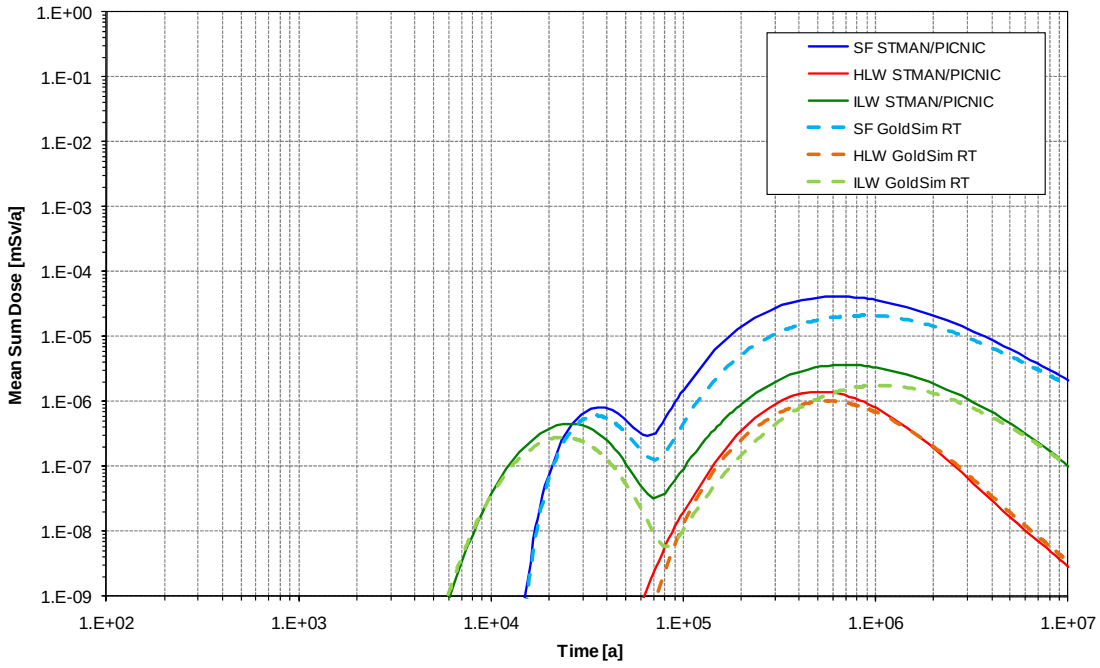

Fig. 6.4-1: Mean doses for SF, HLW and ILW, calculated with STMAN/PICNIC and GoldSim RT.

Tab. 6.4-1: Comparison of maximum mean dose values for SF, HLW and ILW, calculated with STMAN/PICNIC and GoldSim RT.

	Mean sum dose [mSv/a]	
	STMAN/PICNIC	**GoldSim RT**
SF	4.16×10^{-5}	2.13×10^{-5}
HLW	1.42×10^{-6}	1.01×10^{-6}
ILW	3.68×10^{-6}	1.79×10^{-6}

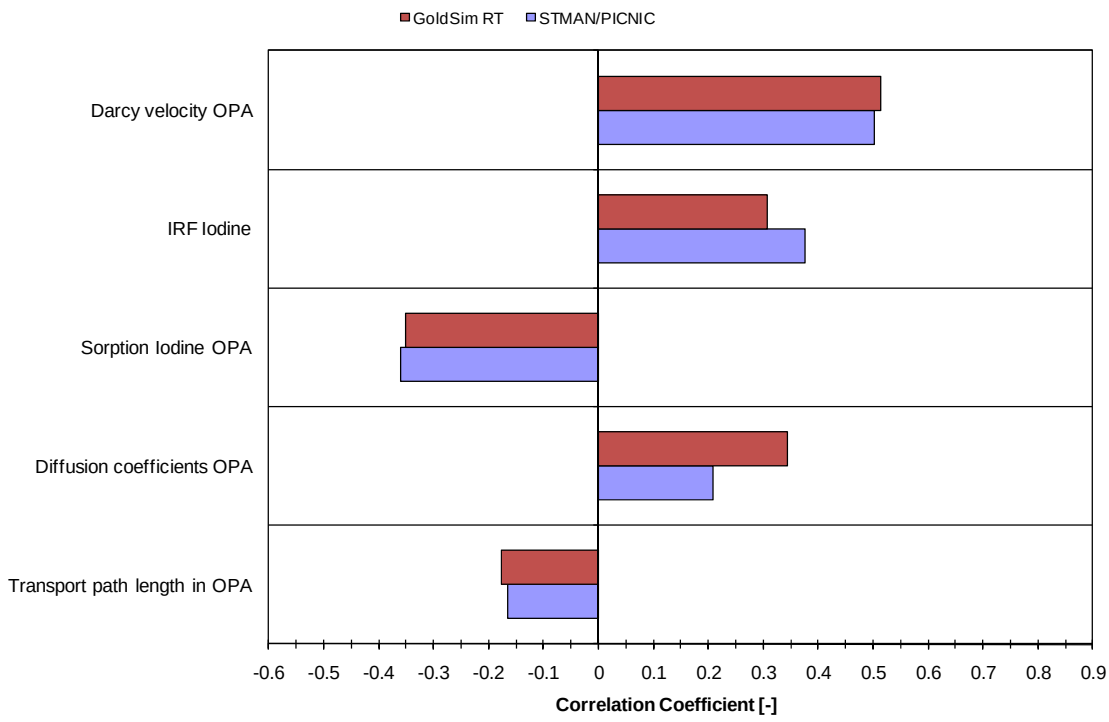

Fig. 6.4-2: Parameter correlation with maximum peak dose for SF, calculated with STMAN/ PICNIC and GoldSim RT.

7 Status, outlook and conclusions

7.1 Status

The main objective of Task 2.2.E was to develop and test an integrated approach for a fully probabilistic safety assessment and the necessary tools. Additional objectives included the realisation of a set of corresponding independent complementary calculations using existing software tools, and a review of the regulatory situation regarding probabilistic safety assessments.

As discussed in Chapter 1.3, the essential first task in the project was the derivation of a comprehensive list of relevant phenomena to be modelled. To ensure that the broad range of uncertainties associated with potentially safety-relevant phenomena would be adequately considered in deriving such a list, the scientists representing the various disciplines were directly involved early on in the project through a clearly defined process. As a result, a list of relevant phenomena to be included in the PSA tools was developed (FEP-Screening Report, Nagra 2007).

The second and most ambitious task of the project was to develop a software package capable of simultaneously modelling all the identified phenomena and their interactions (the *Integrated Radionuclide Release Code IRRC*). As a result of this task, the IRRC is now fully operational (Software Architecture Report, Nagra 2009a), albeit with certain shortcomings. The maximum version that explicitly considers all safety-relevant FEPs (see Chapter 2) is relatively slow. The maximum CPU time[7] required for the *Integrated Flow Code IFC*, with all safety-relevant FEPs included is about 45 hours for a 1 million year period. The remainder of the IRRC calculations take about 40 minutes with all radionuclide processes being considered. A number of preliminary functionality tests have been completed successfully.

The simplified PSA approach has been implemented and tested for spent fuel, vitrified high-level waste, long-lived intermediate-level waste and low- and intermediated level waste (Chapter 4). The independently undertaken complementary calculations for spent fuel, vitrified high-level waste and long-lived intermediate-level waste using GoldSim RT (Chapter 5) show reasonable agreement with those of the simplified modelling using STMAN and PICNIC. Between the two modelling approaches the differences in maximum dose values are about a factor of 2 or less. Since the input parameters used in the two approaches were identical, this difference can be viewed as a measure of the influence of using alternative conceptualisations (1D vs. 2D, different conceptualisation of the interface between the near field and the host rock).

The review of the regulatory situation regarding probabilistic safety assessments was deliberately undertaken (and documented) independently from the PSA development work described above (Röhlig & Plischke 2009).

7.2 Outlook

With many desirable and feasible enhancements in store, the IRRC can now be further developed. Further experience will be gained with running the full IRRC. One task will be to reduce successively the number of FEPs included while continuously monitoring the effect on

[7] The simulation was performed on a Dell laptop, Latitude D620, with an Intel© Corel™ 2 CPU T7600 @ 2.33 GHz and 2 GB of RAM, running under Microsoft Windows XP, Professional, Version 2002, Service Pack 3. The FORTRAN source code was compiled using the Intel® Visual FORTRAN Compiler 9.1.

calculated releases and on the required CPU time. Another task will be to run the IRRC in a fully probabilistic environment using GoldSim as a probabilistic driver and TREETOOL to account for mutually exclusive FEPs. For operational applications it will be necessary to adapt the mesh because the repository design has been further developed in the meantime. Also, an expert elicitation process will be required to obtain the necessary input, e.g. with respect to scenarios, conceptual models and data.

7.3 Conclusions

Nagra started the development of a fully probabilistic approach in the framework of post-closure radiological safety assessment of repositories for spent fuel, vitrified high-level waste and long-lived intermediate-level waste with a Pilot Study in 2006, before the start of the PAMINA project. Within the PAMINA project, as a first step, a comprehensive list of safety-relevant FEPs to be considered was developed in a clearly defined process. The second step involved the successful development of the *Integrated Radionuclide Release Code* IRRC explicitly taking into account all of these FEPs. However, both of these tasks were more difficult and time consuming than originally thought. Regarding the first task, one important factor was the involvement of a large team of experts from many disciplines, with a total of ten specific project meetings dedicated to the development of the list of safety-relevant FEPs. Regarding the second task, we note that:

- the IRRC is a unique tool as it fully incorporates the 52 safety-relevant FEPs (and their interactions), which were derived in a systematic manner,
- the IRRC is therefore a useful research tool in its own right, and
- the IRRC is an excellent basis for further development as it will serve as the key part of a fully probabilistic PSA environment.

One merit of the IRRC is that it allows for the systematic reduction of the number of FEPs included while monitoring the effects on the calculated releases and the CPU time needed. Along the way, benchmarks are obtained "for free" as the scope is trimmed in a step-wise manner from the "maximum version" to the "reduced version".

The simplified PSA approach offers on the one hand a flexibility and robustness which allows PSA to be effectively performed. On the other hand it has the disadvantage that not all identified safety-relevant FEPs can be addressed. While in the future the simplified PSA may be superseded by a fully probabilistic PSA environment making use of the IRRC, until then and for certain applications it may continue to be used for "insight calculations" to complement deterministic calculations.

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Appendix A: List of abbreviations

EDZ	Excavation Disturbed Zone
FEPs	Features, Events and Processes
GoldSim	Monte Carlo simulation software solution for dynamically modelling complex systems, see Chapter 4.1.1
HLW	Vitrified high-level waste
IFC	Integrated Flow Code
IRF	Instant Release Fraction
ILW	Long-lived intermediate-level waste
IRRC	Integrated Radionuclide Release Code
L/ILW	Low- and intermediate-level waste
PICNIC	Geosphere transport code, see Chapter 4.1.4
PSA	Probabilistic Safety Assessment
SF	Spent fuel
SPENT	Source term model for spent fuel used in STMAN.
STALLION	Source term model for low or intermediate level waste used in STMAN.
STMAN	Near field transport code, see Chapter 4.1.2
STRENG	Source term model for high level waste used in STMAN.
VPAC	*Versatile Performance Assessment Code*; flow and transport code for near field and geosphere, see Chapter 4.1.3.

Appendix B: HLW repository input parameters

Tab. B-1: SPENT, STRENG and STALLION input data for the radionuclides and inventory in the Reference Case.

Input	Units	Values
Nuclides and Decays		
Nuclides and decays to be used	Half lives are specified in years	Tab. B-7
Total Inventory		
Inventory of each nuclide for a single package (SF/HLW) or ILW-1 / ILW-2 tunnels	moles or TBq	Tab. B-8 and Tab. B-9

Tab. B-2: SPENT input data for the spent fuel waste form and canister in the Reference Case; values taken from Nagra (2002b).

Input	Units	Values
Inventory Fractions		
Percentage of the inventory for each nuclide for matrix, cladding and instant release	dimensionless (%)	Tab. B-8
Canister Properties		
Containment time	years	10'000
Number of canisters	dimensionless	935 BWR 680 PWR 450 Mixed
Canister length	m	4.6
Initial diameter of waste	m	1.05
Release Properties		
Matrix release rate	per year	Tab. B-10
Grain (or cladding) release rate	per year	3×10^{-5}
Reservoir thickness	m	0.041
Solubility limits	mol/l	Tab. B-11

Tab. B-3: STRENG input data for the vitrified HLW waste form and canister in the Reference Case; values taken from Nagra (2002b).

Input	**Units**	**Values**
Canister Properties		
Containment time	years	10'000
Number of canisters	dimensionless	270 HLW BNFL 460 HLW Cogema
Canister length	m	1.03
Release Properties		
Glass grain density	kg/m^3	2'750
Glass dissolution rate	$kg/(m^2\ a)$	5.5×10^{-4} HLW BNFL 7.3×10^{-5} HLW Cogema
Equivalent spherical radius	m	1.8×10^{-2}
Reservoir thickness	m	0.025
Solubility limits	mol/l	Tab. B-11

Tab. B-4: STALLION input data for the ILW waste form and container in the Reference Case; values taken from Nagra (2002b).

Input	**Units**	**Values**
Waste Package Properties		
Containment time	years	100
Number of waste packages	dimensionless	1 (ILW-) 1 (ILW-2)
Waste package length	m	180 (ILW-1) 60 (ILW-2)
Cementitious Region Properties		
Porosity	dimensionless	0.3
Grain density	kg/m^3	700 (ILW-1) 400 (ILW-2)
Sorption K_d	m^3/kg	Tab. B-12
Solubility limits	mol/l	Tab. B-13

Tab. B-5: SPENT/STRENG input data for the bentonite buffer and STMAN near field / geosphere properties in the Reference Case; values taken from Nagra (2002b).

Input	**Units**	**Values**
Buffer Properties		
Inner radius	m	0.525 (SF) 0.47 (HLW)
Outer radius	m	1.15
Porosity	dimensionless	0.36
Porosity Factors	dimensionless	0.14 (anions) 1 (non-anions)
Grain density	kg/m^3	2760
Sorption K_d	m^3/kg	Tab. B-14
Solubility limits	mol/l	Tab. B-11
Effective diffusion coefficient	m^2/a	Tab. B-14
Interface Near field / Geosphere Properties		
Mixing cell flow rate per waste package	m^3/a	6.0×10^{-3} (SF) 4.0×10^{-3} (HLW) 2.2×10^{-3} (ILW-1) 1.6×10^{-3} (ILW-2)

Tab. B-6: PICNIC input data in the Reference Case; values taken from Nagra (2002b).

Input	**Units**	**Values**
Nuclides and Decays		
Nuclides and decays to be used	Half lives are specified in years.	Tab. B-7
Network Structure		
List of junction names. Inlet and outlet junctions for each leg.	-	Only a single PICNIC leg is considered in the Reference Case, representing a single transport path through the Opalinus Clay
Leg Data – Basic Data		
Length	m	40
Cross-sectional area	m^2	Irrelevant
Darcy velocity	m/a	6.3×10^{-7}
Hydraulic conductivity	m/a	Omitted since specific flow is specified by Darcy velocity
Peclet number	dimensionless	10
Effective diffusion coefficient	m^2/a	Tab. B-15
Leg Data – Properties of Flowing Region		
Retardation	dimensionless	Calculated from the other parameters
Grain density	kg/m^3	2720
Flow porosity	dimensionless	This is set equal to the infill porosity
Infill Porosity	dimensionless	0.12
Porosity Factors	dimensionless	0.5 (anions) 1 (non-anions)
Sorption K_d	m^3/kg	Tab. B-15
Leg Data – Properties of Matrix – Network Flow Data		
There is no "matrix" in the Reference Case – the Opalinus Clay is a homogeneous porous medium. The matrix penetration depth and surface sorption coefficients are thus set equal to zero, and all other parameters are irrelevant. There is no flow "network" in the Reference Case, just 1 single leg.		
Source Term Information		
Source flux	mol/a	Output from STMAN
Fraction to each leg	dimensionless	Only a single PICNIC leg is considered in the Reference Case

Tab. B-7: Safety-relevant radionuclides and properties related to radioactivity; values taken from Nagra (2002b).

Radionuclide and daughters		Half-life [a]	Conversion factor from moles to Bq [Bq/mol]	Dose coefficient		γ-ray exposure factor [Sv/(Bq/m^3) a]
				for inhalation [Sv/Bq]	for ingestion [Sv/Bq]	
Activation / fission products	^{3}H	1.2×10^{1}	1.1×10^{15}	2.6×10^{-10}	4.2×10^{-11}	0.0
	^{10}Be	1.6×10^{6}	8.3×10^{9}	3.5×10^{-9}	1.1×10^{-9}	0.0
	^{14}C	5.7×10^{3}	2.3×10^{12}	5.8×10^{-10}	5.8×10^{-10}	0.0
	^{36}Cl	3.0×10^{5}	4.4×10^{10}	7.3×10^{-10}	9.3×10^{-10}	0.0
	^{41}Ca	1.0×10^{5}	1.3×10^{11}	1.8×10^{-10}	1.9×10^{-10}	0.0
	^{59}Ni	7.5×10^{4}	1.8×10^{11}	4.4×10^{-11}	6.3×10^{-11}	0.0
	^{60}Co → Ni (stable)	5.3×10^{0}	2.5×10^{15}	3.1×10^{-9}	3.4×10^{-9}	2.47×10^{-9}
	^{63}Ni	1.0×10^{2}	1.3×10^{14}	1.3×10^{-10}	1.5×10^{-10}	0.0
	^{79}Se	1.1×10^{6}	1.2×10^{10}	6.8×10^{-9}	2.9×10^{-9}	0.0
	^{90}Sr →Zr (stable)	2.9×10^{1}	4.6×10^{14}	1.6×10^{-8}	3.1×10^{-8}	0.0
	^{93}Mo → ^{93m}Nb	4.0×10^{3}	3.3×10^{12}	2.3×10^{-9}	3.1×10^{-9}	0.0
	^{93m}Nb → Nb (stable)	1.6×10^{1}	8.2×10^{14}	1.8×10^{-10}	1.2×10^{-10}	0.0
	^{93}Zr → ^{93m}Nb (95 %) ^{93}Nb (5 %)	1.5×10^{6}	8.8×10^{9}	2.5×10^{-9}	1.1×10^{-9}	0.0
	^{94}Nb	2.0×10^{4}	6.6×10^{11}	4.9×10^{-9}	1.7×10^{-9}	1.44×10^{-9}
	^{99}Tc	2.1×10^{5}	6.3×10^{10}	1.3×10^{-10}	6.4×10^{-10}	0.0
	^{107}Pd → Ag (stable)	6.5×10^{6}	2.0×10^{9}	5.9×10^{-11}	3.7×10^{-11}	0.0
	^{108m}Ag → Pd (stable)	4.2×10^{2}	3.2×10^{13}	3.7×10^{-9}	2.3×10^{-9}	1.38×10^{-9}
	^{121m}Sn	5.5×10^{1}	2.4×10^{14}	4.7×10^{-10}	5.6×10^{-10}	2.05×10^{-12}
	^{126}Sn	2.3×10^{5}	5.6×10^{10}	2.8×10^{-9}	5.1×10^{-9}	2.65×10^{-11}
	^{129}I	1.6×10^{7}	8.4×10^{8}	3.6×10^{-7}	1.1×10^{-7}	3.08×10^{-12}
	^{135}Cs	2.3×10^{6}	5.8×10^{9}	8.6×10^{-9}	2.0×10^{-9}	0.0
	^{137}Cs	3.0×10^{1}	4.4×10^{14}	3.9×10^{-8}	1.3×10^{-8}	4.91×10^{-10}
	^{151}Sm	9.3×10^{1}	1.4×10^{14}	4.0×10^{-11}	9.8×10^{-11}	2.16×10^{-13}
	^{166m}Ho	1.2×10^{3}	1.1×10^{13}	1.2×10^{-9}	2.0×10^{-9}	1.43×10^{-9}
	^{154}Eu	8.8	1.5×10^{15}	5.3×10^{-9}	2.0×10^{-9}	1.10×10^{-9}

Tab. B-7: (Cont.)

Radionuclide and daughters		Half-life [a]	Conversion factor from moles to Bq [Bq/mol]	Dose coefficient		γ-ray exposure factor [Sv/(Bq/m^3) a]
				for inhalation [Sv/Bq]	for ingestion [Sv/Bq]	
4N chain	^{228}Ra → ^{228}Th	5.8	2.3×10^{15}	1.6×10^{-7}	6.9×10^{-7}	0.0
	^{228}Th → Pb (stable)	1.9	6.9×10^{15}	4.4×10^{-7}	1.4×10^{-7}	1.83×10^{-12}
	^{232}Th → ^{228}Ra	1.4×10^{10}	9.4×10^{5}	1.1×10^{-7}	2.3×10^{-7}	1.31×10^{-13}
	^{232}U → ^{228}Th	6.9×10^{1}	1.9×10^{14}	3.7×10^{-7}	3.3×10^{-7}	5.29×10^{-13}
	^{236}U → ^{232}Th	2.3×10^{7}	5.6×10^{8}	8.7×10^{-8}	4.7×10^{-8}	0.0
	^{240}Pu → ^{236}U	6.6×10^{3}	2.0×10^{12}	1.2×10^{-7}	2.5×10^{-7}	0.0
	^{244}Cm → ^{240}Pu	1.8×10^{1}	7.3×10^{14}	5.7×10^{-7}	1.2×10^{-7}	3.91×10^{-14}
4N+1 chain	^{229}Th → Pb (stable)	7.9×10^{3}	1.7×10^{12}	2.6×10^{-4}	6.1×10^{-7}	1.77×10^{-11}
	^{233}U → ^{229}Th	1.6×10^{5}	8.3×10^{10}	9.6×10^{-6}	5.1×10^{-8}	5.29×10^{-13}
	^{237}Np → ^{233}U	2.1×10^{6}	6.2×10^{9}	5.0×10^{-5}	1.1×10^{-7}	1.62×10^{-11}
	^{241}Am → ^{237}Np	4.3×10^{2}	3.1×10^{13}	9.6×10^{-5}	2.0×10^{-7}	9.48×10^{-12}
	^{241}Pu → ^{241}Am	1.4×10^{1}	9.2×10^{14}	2.3×10^{-6}	4.8×10^{-9}	0.0
	^{245}Cm → ^{241}Pu	8.5×10^{3}	1.6×10^{12}	9.9×10^{-5}	2.1×10^{-7}	2.78×10^{-11}
4N+2 chain	^{210}Pb → ^{210}Po	2.2×10^{1}	5.9×10^{14}	5.7×10^{-6}	6.9×10^{-7}	6.20×10^{-13}
	^{210}Po → Pb (stable)	3.8×10^{-1}	3.5×10^{16}	4.3×10^{-6}	1.2×10^{-6}	5.54×10^{-14}
	^{226}Ra → ^{210}Pb	1.6×10^{3}	8.3×10^{12}	9.5×10^{-6}	2.8×10^{-7}	5.49×10^{-12}
	^{230}Th → ^{226}Ra	7.5×10^{4}	1.8×10^{11}	1.0×10^{-4}	2.1×10^{-7}	3.02×10^{-13}
	^{234}U → ^{230}Th	2.5×10^{5}	5.4×10^{10}	9.4×10^{-6}	4.9×10^{-8}	2.70×10^{-13}
	^{238}Pu → ^{234}U	8.8×10^{1}	1.5×10^{14}	1.1×10^{-4}	2.3×10^{-7}	1.16×10^{-13}
	^{238}U → ^{234}U	4.5×10^{9}	3.0×10^{6}	8.0×10^{-6}	4.8×10^{-8}	0.0
	^{242m}Am → ^{238}Pu (82.7 %) ^{242}Pu (17.3 %)	1.4×10^{2}	9.4×10^{13}	9.7×10^{-5}	2.0×10^{-7}	0.0
	^{242}Pu → ^{238}U	3.8×10^{5}	3.5×10^{10}	1.1×10^{-4}	2.4×10^{-7}	0.0
	^{246}Cm → ^{242}Pu	4.7×10^{3}	2.8×10^{12}	9.8×10^{-5}	2.1×10^{-7}	0.0
4N+3 chain	^{227}Ac → Pb (stable)	2.2×10^{1}	6.1×10^{14}	5.7×10^{-4}	1.2×10^{-6}	0.0
	^{231}Pa → ^{227}Ac	3.3×10^{4}	4.0×10^{11}	1.4×10^{-4}	7.1×10^{-7}	1.60×10^{-11}
	^{235}U → ^{231}Pa	7.0×10^{8}	1.9×10^{7}	8.5×10^{-6}	4.7×10^{-8}	9.49×10^{-11}
	^{239}Pu → ^{235}U	2.4×10^{4}	5.5×10^{11}	1.2×10^{-4}	2.5×10^{-7}	5.75×10^{-14}
	^{243}Am → ^{239}Pu	7.4×10^{3}	1.8×10^{12}	9.6×10^{-5}	2.0×10^{-7}	2.56×10^{-11}
	^{243}Cm → ^{239}Pu	2.9×10^{1}	4.5×10^{14}	6.9×10^{-5}	1.5×10^{-7}	3.91×10^{-14}

Tab. B-8: Inventories and their distributions – reference SF packages; values taken from Nagra (2002b).

Radionuclides and stable isotopes		Inventory per waste package after 40 years decay [mol] and distribution [%]								
		BWR-UO_2-48			PWR-mixed-48			PWR-UO_2-48		
		matrix	clad.	IRF	matrix	clad.	IRF	matrix	clad.	IRF
Activation / fission products	^{3}H	6.53×10^{-3}			6.10×10^{-3}			6.38×10^{-3}		
		98	0	2	98	0	2	98	0	2
	^{10}Be	2.12×10^{-3}			2.03×10^{-3}			2.07×10^{-3}		
		90	0	10	90	0	10	90	0	10
	$^{14}C_{inorg}$	2.89×10^{-2}			2.41×10^{-2}			2.70×10^{-2}		
		90	0	10	90	0	10	90	0	10
	$^{14}C_{org}$	2.48×10^{-2}			1.36×10^{-2}			1.55×10^{-2}		
		0	80	20	0	80	20	0	80	20
	^{36}Cl	5.17×10^{-2}			3.16×10^{-2}			3.70×10^{-2}		
		33	62	5	44	51	5	45	50	5
	^{41}Ca	2.28×10^{-3}			1.70×10^{-3}			2.01×10^{-3}		
		76	24	0	84	16	0	84	16	0
	^{59}Ni	7.20×10^{-1}			6.62×10^{-1}			6.91×10^{-1}		
		1	99	0	1	99	0	1	99	0
	^{63}Ni	1.03×10^{-1}			9.45×10^{-2}			1.01×10^{-1}		
		1	99	0	1	9	0	1	99	0
	^{79}Se	1.32×10^{-1}			1.21×10^{-1}			1.29×10^{-1}		
		91	0	9	94	0	6	96	0	4
	^{90}Sr	4.83			4.07			4.72		
		99	0	1	99	0	1	99	0	1
	^{93}Mo	1.26×10^{-4}			2.36×10^{-4}			2.44×10^{-4}		
		20	80	0	9	91	0	9	91	0
	^{93m}Nb	1.61×10^{-4}			1.38×10^{-4}			1.53×10^{-4}		
		89	11	0	93	7	0	93	7	0
	^{93}Zr	1.90×10^{2}			1.61×10^{2}			1.80×10^{2}		
		90	10	0	93	7	0	93	7	0
	^{94}Nb	2.00×10^{-2}			5.46×10^{-2}			5.67×10^{-2}		
		2	98	0	0	100	0	0	100	0
	^{99}Tc	1.77×10^{1}			1.65×10^{1}			1.73×10^{1}		
		98	0	2	98	0	2	98	0	2
	^{107}Pd	5.00			5.62			4.74		
		98	0	2	98	0	2	98	0	2
	^{108m}Ag	4.58×10^{-5}			3.89×10^{-5}			4.23×10^{-5}		
		100	0	0	100	0	0	100	0	0

Tab. B-8: (Cont.)

Radionuclides and stable isotopes		Inventory per waste package after 40 years decay [mol] and distribution [%]								
		BWR-UO_2-48			PWR-mixed-48			PWR-UO_2-48		
		matrix	clad.	IRF	matrix	clad.	IRF	matrix	clad.	IRF
Activation / fission products	^{126}Sn	5.36×10^{-1}			5.89×10^{-1}			5.24×10^{-1}		
		91	0	9	92	0	8	96	0	4
	^{129}I	3.21			3.17			3.14		
		91	0	9	93	0	7	96	0	4
	^{135}Cs	6.37			7.56			6.76		
		95	0	5	94	0	6	96	0	4
	^{137}Cs	7.99			7.49			7.79		
		95	0	5	95	0	5	96	0	4
	^{151}Sm	1.12×10^{-1}			1.32×10^{-1}			1.10×10^{-1}		
		100	0	0	100	0	0	100	0	0
	^{166m}Ho	1.88×10^{-4}			1.83×10^{-4}			1.70×10^{-4}		
		100	0	0	100	0	0	100	0	0
Stable isotopes	Ag	1.60			1.92			1.56		
		100	0	0	100	0	0	100	0	0
	Ca	2.31			1.99			2.08		
		78	22	0	85	15	0	85	15	0
	Ho	5.89×10^{-3}			6.85×10^{-3}			5.75×10^{-3}		
		100	0	0	100	0	0	100	0	0
	Nb	1.39			6.16			6.35		
		1	99	0	0	100	0	0	100	0
	Ni	2.63×10^{2}			3.98×10^{2}			4.12×10^{2}		
		0	100	0	0	100	0	0	100	0
	Pb	4.35×10^{-1}			2.61×10^{-1}			2.75×10^{-1}		
		2	98	0	3	97	0	3	97	0
	Pd	2.43×10^{1}			2.61×10^{1}			2.34×10^{1}		
		98	0	2	98	0	2	98	0	2
	Se	1.40			1.25			1.38		
		91	0	9	94	0	6	96	0	4
	Sm	6.91			6.48			6.58		
		100	0	0	100	0	0	100	0	0
	Sn	8.68×10^{1}			5.20×10^{1}			5.48×10^{1}		
		1	99	0	2	98	0	1	99	0
	Sr	8.28			7.09			8.24		
		99	0	1	99	0	1	99	0	1
	Zr	7.38×10^{3}			4.46×10^{3}			4.71×10^{3}		
		1	99	0	1	99	0	2	98	0

Tab. B-8: (Cont.)

Radionuclides and stable isotopes		Inventory per waste package after 40 years decay [mol] and distribution [%]								
		BWR-UO_2-48			PWR-mixed-48			PWR-UO_2-48		
		matrix	clad.	IRF	matrix	clad.	IRF	matrix	clad.	IRF
4N chain	^{228}Ra	1.38×10^{-14}			1.03×10^{-14}			1.35×10^{-14}		
		100	0	0	100	0	0	100	0	0
	^{228}Th	2.76×10^{-8}			2.40×10^{-8}			2.92×10^{-8}		
		100	0	0	100	0	0	100	0	0
	^{232}Th	4.40×10^{-5}			3.29×10^{-5}			4.29×10^{-5}		
		100	0	0	100	0	0	100	0	0
	^{232}U	9.12×10^{-7}			8.65×10^{-7}			1.05×10^{-6}		
		100	0	0	100	0	0	100	0	0
	^{236}U	3.67×10^{1}			2.74×10^{1}			3.58×10^{1}		
		100	0	0	100	0	0	100	0	0
	^{240}Pu	1.97×10^{1}			3.25×10^{1}			1.78×10^{1}		
		100	0	0	100	0	0	100	0	0
	^{244}Cm	1.09×10^{-1}			2.49×10^{-1}			1.02×10^{-1}		
		100	0	0	100	0	0	100	0	0
4N+1 chain	^{229}Th	8.46×10^{-9}			6.79×10^{-9}			8.46×10^{-9}		
		100	0	0	100	0	0	100	0	0
	^{233}U	8.04×10^{-5}			6.51×10^{-5}			7.86×10^{-5}		
		100	0	0	100	0	0	100	0	0
	^{237}Np	5.15			4.47			5.04		
		100	0	0	100	0	0	100	0	0
	^{241}Am	9.87			1.60×10^{1}			9.15		
		100	0	0	100	0	0	100	0	0
	^{241}Pu	1.66			2.67			1.58		
		100	0	0	100	0	0	100	0	0
	^{245}Cm	3.58×10^{-2}			1.13×10^{-1}			3.20×10^{-2}		
		100	0	0	100	0	0	100	0	0
4N+2 chain	^{210}Pb	1.58×10^{-10}			1.40×10^{-10}			1.70×10^{-10}		
		100	0	0		100	0	0		100
	^{210}Po	2.60×10^{-12}			2.30×10^{-12}			2.81×10^{-12}		
		100	0	0		100	0	0		100
	^{226}Ra	3.46×10^{-8}			3.15×10^{-8}			3.76×10^{-8}		
		100	0	0		100	0	0		100
	^{230}Th	1.81×10^{-4}			1.71×10^{-4}			1.95×10^{-4}		
		100	0	0		100	0	0		100

Tab. B-8: (Cont.)

Radionuclides and stable isotopes		Inventory per waste package after 40 years decay [mol] and distribution [%]								
		BWR-UO_2-48			PWR-mixed-48			PWR-UO_2-48		
		matrix	clad.	IRF	matrix	clad.	IRF	matrix	clad.	IRF
4N+2 chain	^{234}U	1.80			1.77			1.85		
		100	0	0		100	0	0		100
	^{238}Pu	1.69			2.13			1.55		
		100	0	0		100	0	0		100
	^{238}U	6.45×10^{3}			5.54×10^{3}			5.78×10^{3}		
		100	0	0		100	0	0		100
	^{242m}Am	6.06×10^{-3}			2.48×10^{-2}			6.58×10^{-3}		
		100	0	0		100	0	0		100
	^{242}Pu	5.41			8.68			4.85		
		100	0	0		100	0	0		100
	^{246}Cm	4.33×10^{-3}			1.17×10^{-2}			4.11×10^{-3}		
		100	0	0		100	0	0		100
4N+3 chain	^{227}Ac	5.50×10^{-10}			5.00×10^{-10}			6.40×10^{-10}		
		100	0	0		100	0	0		100
	^{231}Pa	1.89×10^{-6}			1.74×10^{-6}			2.23×10^{-6}		
		100	0	0		100	0	0		100
	^{235}U	4.83×10^{1}			4.46×10^{1}			5.69×10^{1}		
		100	0	0		100	0	0		100
	^{239}Pu	4.06×10^{1}			5.23×10^{1}			3.97×10^{1}		
		100	0	0		100	0	0		100
	^{243}Am	1.24			2.21			1.13		
		100	0	0		100	0	0		100
	^{243}Cm	1.47×10^{-3}			4.33×10^{-3}			1.44×10^{-3}		
		100	0	0		100	0	0		100

Tab. B-9: Reference inventories of HLW packages and ILW tunnels; values taken from Nagra (2002b).

Radionuclides and stable isotopes		Inventory per waste package after 40 years decay [mol]		Total inventory after 40 years decay [mol]	
		Reference inventory			
		COGEMA	BNFL	ILW-1	ILW-2
Activation / fission products	^{3}H	-	-	2.01	3.92×10^{-5}
	$^{14}C_{inorg}$	8.23×10^{-5}	3.08×10^{-5}	4.00	-
	$^{14}C_{org}$	-	-	3.94	3.48×10^{-4}
	^{36}Cl	-	-	1.43	3.56×10^{-4}
	^{59}Ni	1.36×10^{-2}	3.80×10^{-3}	6.96×10^{2}	3.91×10^{-3}
	^{60}Co	-	-	1.61×10^{-1}	7.94×10^{-6}
	^{63}Ni	1.99×10^{-3}	5.42×10^{-4}	1.11×10^{2}	5.26×10^{-4}
	^{79}Se	9.98×10^{-2}	1.33×10^{-1}	1.12×10^{-1}	7.64×10^{-4}
	^{90}Sr	2.81	3.46	4.45	1.66×10^{-2}
	^{93}Mo	1.54×10^{-5}	1.51×10^{-5}	4.30×10^{-1}	8.16×10^{-7}
	^{93m}Nb	9.39×10^{-5}	1.34×10^{-4}	7.33×10^{-3}	1.03×10^{-4}
	^{93}Zr	1.07×10^{2}	1.47×10^{2}	6.70×10^{3}	1.17×10^{2}
	^{94}Nb	1.03×10^{-3}	1.50×10^{-5}	4.78×10^{1}	9.83×10^{-6}
	^{99}Tc	1.33×10^{1}	1.49×10^{1}	2.54×10^{1}	6.08×10^{-2}
	^{107}Pd	3.19	3.69	-	-
	^{108m}Ag	1.71×10^{-5}	1.49×10^{-5}	-	-
	^{121m}Sn	6.56×10^{-1}	-	1.09	1.75×10^{-6}
	^{126}Sn	-	9.04×10^{-1}	2.79×10^{-1}	5.23×10^{-2}
	^{129}I	1.90×10^{-3}	2.49×10^{-3}	5.13×10^{1}	4.55
	^{135}Cs	3.48	6.78	2.08×10^{1}	5.13×10^{-2}
	^{137}Cs	4.33	5.25	9.76	7.34×10^{-2}
	^{151}Sm	9.84×10^{-2}	1.20×10^{-1}	3.72×10^{-1}	1.80×10^{-3}
	^{154}Eu	-	-	2.09×10^{-2}	1.63×10^{-4}
	^{166m}Ho	1.63×10^{-5}	1.36×10^{-5}	-	-
Stable is.	Ni	1.07×10^{1}	5.71	-	-
	Pd	1.74×10^{1}	1.94×10^{1}	-	-
	Se	8.88×10^{-1}	1.22	-	-
	Sn	1.08	9.71×10^{-1}	-	-

Tab. B-9: (Cont.)

Radionuclides and stable isotopes		Inventory per waste package after 40 years decay [mol]		Total inventory after 40 years decay [mol]	
		Reference inventory			
		COGEMA	BNFL	ILW-1	ILW-2
4N chain	^{228}Ra	1.17×10^{-17}	2.43×10^{-18}	0	0
	^{228}Th	1.59×10^{-10}	3.33×10^{-11}	2.30×10^{-8}	0
	^{232}Th	3.61×10^{-8}	7.54×10^{-9}	0	0
	^{232}U	5.21×10^{-9}	1.20×10^{-9}	8.14×10^{-7}	0
	^{236}U	3.01×10^{-2}	6.55×10^{-3}	1.35×10^{1}	2.17
	^{240}Pu	9.43×10^{-2}	1.14×10^{-1}	1.17×10^{1}	3.80×10^{-1}
	^{244}Cm	2.05×10^{-2}	1.64×10^{-2}	7.35×10^{-3}	1.36×10^{-4}
4N+1 chain	^{229}Th	3.28×10^{-9}	3.75×10^{-9}	2.06×10^{-9}	0
	^{233}U	3.73×10^{-5}	4.21×10^{-5}	2.18×10^{-5}	9.22×10^{-7}
	^{237}Np	2.76	3.24	1.20	8.07×10^{-2}
	^{241}Am	1.01	3.27	5.37	2.25×10^{-1}
	^{241}Pu	9.66×10^{-4}	2.39×10^{-3}	6.27×10^{-1}	3.37×10^{-2}
	^{245}Cm	3.79×10^{-3}	4.18×10^{-3}	9.73×10^{-4}	2.36×10^{-5}
	^{210}Pb	3.88×10^{-11}	1.37×10^{-10}	7.93×10^{-11}	1.03×10^{-11}
	^{210}Po	6.30×10^{-13}	2.26×10^{-12}	1.30×10^{-12}	$1.76 \times 10\text{-}^{13}$
4N+2 chain	^{226}Ra	6.53×10^{-9}	2.30×10^{-8}	1.85×10^{-8}	2.41×10^{-9}
	^{230}Th	1.77×10^{-5}	6.27×10^{-5}	1.05×10^{-4}	1.33×10^{-5}
	^{234}U	1.86×10^{-3}	1.84×10^{-3}	1.02	1.21×10^{-1}
	^{238}Pu	2.06×10^{-3}	5.11×10^{-3}	5.06×10^{-1}	2.54×10^{-2}
	^{238}U	6.42	2.03	3.68×10^{3}	4.91×10^{2}
	^{242m}Am	6.35×10^{-3}	1.27×10^{-2}	1.09×10^{-3}	1.62×10^{-4}
	^{242}Pu	3.12×10^{-3}	9.92×10^{-3}	2.16	1.19×10^{-1}
	^{246}Cm	3.93×10^{-4}	4.29×10^{-4}	1.10×10^{-4}	2.33×10^{-6}
4N+3 chain	^{227}Ac	1.04×10^{-9}	2.63×10^{-9}	6.05×10^{-10}	6.93×10^{-11}
	^{231}Pa	2.06×10^{-6}	4.95×10^{-6}	2.06×10^{-6}	2.37×10^{-7}
	^{235}U	6.38×10^{-2}	1.60×10^{-2}	5.30×10^{1}	5.91
	^{239}Pu	3.83×10^{-2}	1.22×10^{-1}	3.10×10^{1}	1.19
	^{243}Am	4.23×10^{-1}	4.90×10^{-1}	2.01×10^{-1}	2.05×10^{-2}
	^{243}Cm	5.94×10^{-4}	6.38×10^{-4}	2.03×10^{-4}	3.54×10^{-6}

Tab. B-10: Fuel matrix fractional dissolution rate as a function of time, evaluated assuming two different canister loadings; values taken from Nagra (2002b).

Time [a]	**Fuel matrix fractional dissolution rate [1/a]**		
0	1.0×10^{-4}		
50	2.0×10^{-5}		
100	1.5×10^{-5}		
200	1.3×10^{-5}		
300	9.3×10^{-6}		
500	7.2×10^{-6}		
700	5.3×10^{-6}		
	Values based on UO_2 fuel elements with a burn-up of 48 GWd/t_{IHM}	Values based on a weighted average of 1 MOX fuel element and 3 UO_2 fuel elements, each with a burn-up of 48 GWd/t_{IHM}	Values based on MOX fuel elements with a burn-up of 65 GWd/t_{IHM}
1.0×10^{3}	2.4×10^{-6}	3.8×10^{-6}	8.6×10^{-6}
2.0×10^{3}	1.3×10^{-6}	2.0×10^{-6}	4.4×10^{-6}
3.0×10^{3}	8.9×10^{-7}	1.4×10^{-6}	3.1×10^{-6}
5.1×10^{3}	6.7×10^{-7}	1.0×10^{-6}	2.3×10^{-6}
7.6×10^{3}	5.9×10^{-7}	8.9×10^{-7}	1.9×10^{-6}
1.0×10^{4}	5.3×10^{-7}	7.9×10^{-7}	1.7×10^{-6}
1.5×10^{4}	4.2×10^{-7}	6.1×10^{-7}	1.3×10^{-6}
2.0×10^{4}	3.3×10^{-7}	4.7×10^{-7}	9.3×10^{-7}
3.0×10^{4}	2.1×10^{-7}	2.8×10^{-7}	5.3×10^{-7}
5.1×10^{4}	1.1×10^{-7}	1.4×10^{-7}	2.3×10^{-7}
6.4×10^{4}	7.6×10^{-8}	9.8×10^{-8}	1.7×10^{-7}
8.1×10^{4}	5.6×10^{-8}	7.3×10^{-8}	1.3×10^{-7}
1.1×10^{5}	4.0×10^{-8}	5.4×10^{-8}	1.0×10^{-7}
1.5×10^{5}	3.0×10^{-8}	4.2×10^{-8}	8.3×10^{-8}
2.1×10^{5}	2.7×10^{-8}	3.7×10^{-8}	7.4×10^{-8}
3.1×10^{5}	2.5×10^{-8}	3.4×10^{-8}	6.6×10^{-8}
5.2×10^{5}	2.2×10^{-8}	2.9×10^{-8}	5.5×10^{-8}
8.2×10^{5}	1.8×10^{-8}	2.4×10^{-8}	4.5×10^{-8}
1.0×10^{6}	1.6×10^{-8}	2.1×10^{-8}	4.0×10^{-8}
1.6×10^{6}	1.3×10^{-8}	1.8×10^{-8}	3.2×10^{-8}
2.1×10^{6}	1.2×10^{-8}	1.6×10^{-8}	2.7×10^{-8}
3.1×10^{6}	1.1×10^{-8}	1.3×10^{-8}	2.1×10^{-8}
4.9×10^{6}	1.0×10^{-8}	1.1×10^{-8}	1.5×10^{-8}
7.0×10^{6}	1.0×10^{-8}	1.1×10^{-8}	1.2×10^{-8}
$\geq 1.0 \times 10^{7}$	1.0×10^{-8}	1.0×10^{-8}	1.0×10^{-8}

Tab. B-11: Solubility limits and associated uncertainties for the SF / HLW near field; values taken from Nagra (2002a).

Reference Case (pH = 7.25, Eh = -194 mV).

Element	**Reference Case [mol/l]**	**Lower limit (optimistic) [mol/l]**	**Upper limit (pessimistic) [mol/l]**
H	high	high	high
Be	1×10^{-6}	1×10^{-6}	high
C_{inorg}	3×10^{-3}	6×10^{-4}	7×10^{-3}
C_{org}	high	high	high
Cl	high	high	high
Ca	1×10^{-2}	1×10^{-2}	1×10^{-2}
Ni	3×10^{-5}	1×10^{-5}	8×10^{-5}
Se	5×10^{-9}	2×10^{-11}	1×10^{-5}
Sr	2×10^{-5}	3×10^{-6}	1×10^{-4}
Zr	2×10^{-9}	3×10^{-11}	2×10^{-9}
Nb	3×10^{-5}	1×10^{-8}	1×10^{-4}
Mo	1×10^{-6}	1×10^{-6}	1×10^{-5}
Tc	4×10^{-9}	1×10^{-9}	1×10^{-8}
Pd	5×10^{-8}	1×10^{-10}	2×10^{-7}
Ag	3×10^{-6}	1×10^{-10}	3×10^{-6}
Sn	1×10^{-8}	5×10^{-9}	1×10^{-7}
I	high	high	high
Cs	high	high	high
Sm	5×10^{-7}	3×10^{-7}	9×10^{-7}
Ho	5×10^{-7}	3×10^{-7}	9×10^{-7}
Pb	2×10^{-6}	2×10^{-8}	8×10^{-5}
Po	high	high	high
Ra	2×10^{-11}	4×10^{-12}	5×10^{-8}
Ac	1×10^{-6}	5×10^{-8}	3×10^{-5}
Th	7×10^{-7}	2×10^{-7}	3×10^{-6}
Pa	1×10^{-8}	1×10^{-8}	1×10^{-5}
U	3×10^{-9}	3×10^{-10}	5×10^{-7}
Np	5×10^{-9}	3×10^{-9}	1×10^{-8}
Pu	5×10^{-8}	3×10^{-9}	1×10^{-6}
Am	1×10^{-6}	5×10^{-8}	3×10^{-5}
Cm	1×10^{-6}	5×10^{-8}	3×10^{-5}

Tab. B-12: Sorption values (K_d) in cement for the waste groups ILW-1 and ILW-2; values taken from Nagra (2002a).

Reference Cases and corresponding lower (pessimistic) and upper (optimistic) limits.

Element	K_d ILW-1			K_d ILW-2		
	Ref. Case [m^3/kg]	**Lower limit (pessimistic) [m^3/kg]**	**Upper limit (optimistic) [m^3/kg]**	**Ref. Case [m^3/kg]**	**Lower limit (pessimistic) [m^3/kg]**	**Upper limit (optimistic) [m^3/kg]**
H	1×10^{-4}	7×10^{-5}	1 × 10-4	1×10^{-4}	7 × 10-5	1×10^{-4}
C_{inorg}	0	0	0	0	0	0
C_{org}	0	0	0	0	0	0
Cl	0.005	0.003	0.007	0.005	0.003	0.007
Co	0	0	0	0	0	0
Ni	0	0	0	0	0	0
Se	0.03	0.02	0.04	0.001	7×10^{-4}	0.001
Sr	0.001	7×10^{-4}	0.001	0.001	7×10^{-4}	0.001
Zr	10	2	30	10	2	30
Nb	1	0.7	1	1	0.7	1
Mo	0	0	0	0	0	0
Tc	0.001	7×10^{-4}	1	0.001	7×10^{-4}	0.001
Sn	10	2	30	10	2	30
I	0.001	7×10^{-4}	0.001	0.001	7×10^{-4}	0.001
Cs	5×10^{-4}	3×10^{-4}	7×10^{-4}	5×10^{-4}	3×10^{-4}	7×10^{-4}
Sm	80	20	300	80	20	300
Eu	80	20	300	80	20	300
Pb	0.5	0.3	0.7	0.5	0.3	0.7
Po	0	0	0	0	0	0
Ra	0.05	0.03	0.07	0.05	0.03	0.07
Ac	80	20	300	80	20	300
Th	80	20	300	80	20	300
Pa	0.1	0.07	0.1	0.1	0.07	0.1
U	2	1	2	2	1	2
Np	80	20	300	0.1	0.07	0.1
Pu	80	20	300	0.1	0.07	0.1
Am	80	20	300	80	20	300
Cm	80	20	300	80	20	300

Tab. B-13: Solubility limits and associated uncertainties for the cementitious near field of the waste groups ILW-1 and ILW-2; values taken from Nagra (2002a).

Element	ILW-1			ILW-2		
	Ref. Case [mol/l]	**Lower limit (optimistic) [mol/l]**	**Upper limit (pessimistic) [mol/l]**	**Ref. Case [mol/l]**	**Lower limit (optimistic) [mol/l]**	**Upper limit (pessimistic) [mol/l]**
H	high	high	high	high	high	high
C_{inorg}	2×10^{-4}	1×10^{-4}	4×10^{-4}	2×10^{-4}	1×10^{-4}	4×10^{-4}
C_{org}	high	high	high	high	high	high
Cl	high	high	high	high	high	high
Co	7×10^{-7}	7×10^{-7}	7×10^{-6}	high	high	high
Ni	3×10^{-7}	1×10^{-8}	8×10^{-6}	high	high	high
Se	1×10^{-5}	7×10^{-6}	7×10^{-4}	high	high	high
Sr	3×10^{-3}	2×10^{-3}	6×10^{-3}	3×10^{-3}	2×10^{-3}	6×10^{-3}
Zr	6×10^{-6}	6×10^{-7}	6×10^{-5}	6×10^{-6}	6×10^{-7}	6×10^{-5}
Nb	high	high	high	high	high	high
Mo	3×10^{-5}	3×10^{-6}	2×10^{-3}	3×10^{-5}	3×10^{-6}	2×10^{-3}
Tc	high	3×10^{-7}	high	high	high	high
Sn	1×10^{-7}	1×10^{-7}	8×10^{-6}	1×10^{-7}	1×10^{-7}	8×10^{-6}
I	high	high	high	high	high	high
Cs	high	high	high	high	high	high
Sm	2×10^{-6}	2×10^{-7}	2×10^{-5}	2×10^{-6}	2×10^{-7}	2×10^{-5}
Eu	2×10^{-6}	2×10^{-7}	2×10^{-5}	2×10^{-6}	2×10^{-7}	2×10^{-5}
Pb	3×10^{-3}	3×10^{-3}	high	3×10^{-3}	3×10^{-3}	high
Po	high	high	high	high	high	high
Ra	1×10^{-5}	1×10^{-6}	2×10^{-5}	1×10^{-5}	1×10^{-6}	2×10^{-5}
Ac	2×10^{-6}	2×10^{-7}	2×10^{-5}	2×10^{-6}	2×10^{-7}	2×10^{-5}
Th	3×10^{-9}	8×10^{-10}	1×10^{-8}	3×10^{-9}	8×10^{-10}	1×10^{-8}
Pa	1×10^{-8}	1×10^{-8}	high	1×10^{-8}	1×10^{-8}	high
U	1×10^{-8}	1×10^{-8}	5×10^{-7}	1×10^{-8}	1×10^{-8}	5×10^{-7}
Np	5×10^{-9}	3×10^{-9}	1×10^{-8}	high	high	high
Pu	4×10^{-11}	1×10^{-11}	1×10^{-10}	6×10^{-11}	2×10^{-11}	6×10^{-10}
Am	2×10^{-9}	3×10^{-10}	1×10^{-8}	2×10^{-9}	3×10^{-10}	1×10^{-8}
Cm	2×10^{-9}	3×10^{-10}	1×10^{-8}	2×10^{-9}	3×10^{-10}	1×10^{-8}

Tab. B-14: Sorption values (K_d), effective diffusion coefficients (D_e) and accessible porosities (ε) in compacted bentonite; values taken from Nagra (2002a).

Reference Case (pH = 7.25, Eh = -194 mV) including lower (pessimistic) and upper (optimistic) limits.

Element	K_d			D_e	ε
	Ref. Case [m^3/kg]	Lower limit (pessimistic) [m^3/kg]	Upper limit (optimistic) [m^3/kg]	[m^2/s]	[-]
H	0	0	0	2×10^{-10}	0.36
Be	0.2	0.009	5	2×10^{-10}	0.36
C_{inorg}	6×10^{-5}	2×10^{-5}	3×10^{-4}	3×10^{-12}	0.05
C_{org}	0	0	0	2×10^{-10}	0.36
Cl	0	0	0	3×10^{-12}	0.05
Ca	0.003	5×10^{-4}	0.02	2×10^{-10}	0.36
Ni	0.2	0.009	5	2×10^{-10}	0.36
Se	0	0	0	3×10^{-12}	0.05
Sr	0.003	5×10^{-4}	0.02	2×10^{-10}	0.36
Zr	80	1	4000	2×10^{-10}	0.36
Nb	30	1	900	2×10^{-10}	0.36
Mo	0	0	0	3×10^{-12}	0.05
Tc	60	0.5	600	2×10^{-10}	0.36
Pd	5	0.2	100	2×10^{-10}	0.36
Ag	0	0	0	2×10^{-10}	0.36
Sn	800	1	10000	2×10^{-10}	0.36
I	5×10^{-4}	5×10^{-5}	0.005	3×10^{-12}	0.05
Cs	0.1	0.03	0.3	2×10^{-10}	0.36
Sm	4	0.1	100	2×10^{-10}	0.36
Ho	4	0.1	100	2×10^{-10}	0.36
Pb	7	0.5	100	2×10^{-10}	0.36
Po	0.06	0.008	0.5	3×10^{-12}	0.05
Ra	0.002	3×10^{-4}	0.01	2×10^{-10}	0.36
Ac	20	1	300	2×10^{-10}	0.36
Th	60	10	200	2×10^{-10}	0.36
Pa	5	0.2	100	2×10^{-10}	0.36
U	40	2	400	2×10^{-10}	0.36
Np	60	6	600	2×10^{-10}	0.36
Pu	20	1	300	2×10^{-10}	0.36
Am	20	1	300	2×10^{-10}	0.36
Cm	20	1	300	2×10^{-10}	0.36

Tab. B-15: Sorption values (K_d), effective diffusion coefficients (D_e) and accessible porosities (ε) in Opalinus Clay; values taken from Nagra (2002a).

Reference Case (pH = 7.25, Eh = -167 mV) incl. lower (pessimistic) and upper (optimistic) limits for K_d and upper (pessimistic) limits for $D_{e\perp}$ (perpendicular to bedding). In addition, diffusion coefficients parallel to bedding ($D_{e=}$) are given.

Element	K_d			$D_{e\perp}$		$D_{e=}$	ε	Remarks
	Ref. Case [m^3/kg]	Lower limit (pessimistic) [m^3/kg]	Upper limit (optimistic) [m^3/kg]	Ref. Case [m^2/s]	Upper limit (pessimistic) [m^2/s]	[$m^2\ s^{-1}$]	[-]	
H	0	0	0	1×10^{-11}	1×10^{-10}	5×10^{-11}	0.12	
Be	0.9	0.03	20	1×10^{-11}	1×10^{-10}	5×10^{-11}	0.12	
C_{inorg}	0.001	1×10^{-4}	0.006	1×10^{-12}	3×10^{-12}	5×10^{-12}	0.06	Anion
C_{org}	0	0	0	1×10^{-11}	1×10^{-10}	5×10^{-11}	0.12	
Cl	0	0	0	1×10^{-12}	3×10^{-12}	5×10^{-12}	0.06	Anion
Ca	0.001	$1 \times 1^{0-4}$	0.007	1×10^{-11}	1×10^{-10}	5×10^{-11}	0.12	
Co	0.4	0.01	20	1×10^{-11}	1×10^{-10}	5×10^{-11}	0.12	
Ni	0.9	0.03	20	1×10^{-11}	1×10^{-10}	5×10^{-11}	0.12	
Se	0	0	0	1×10^{-12}	3×10^{-12}	5×10^{-12}	0.06	Anion
Sr	0.001	1×10^{-4}	0.007	1×10^{-11}	1×10^{-10}	5×10^{-11}	0.12	
Zr	10	0.3	300	1×10^{-11}	1×10^{-10}	5×10^{-11}	0.12	
Nb	4	0.1	100	1×10^{-11}	1×10^{-10}	5×10^{-11}	0.12	
Mo	0.01	0.001	0.2	1×10^{-12}	3×10^{-12}	5×10^{-12}	0.06	Anion
Tc	50	0.5	500	1×10^{-11}	1×10^{-10}	$5 \times {}^{10}$-11	0.12	
Pd	5	0.2	100	1×10^{-11}	1×10^{-10}	5×10^{-11}	0.12	
Ag	0	0	0	1×10^{-11}	1×10^{-10}	5×10^{-11}	0.12	
Sn	100	0.2	1000	1×10^{-11}	1×10^{-10}	5 × 10-11	0.12	
I	3×10^{-5}	3×10^{-6}	4×10^{-4}	1×10^{-12}	3×10^{-12}	5×10^{-12}	0.06	Anion
Cs	0.5	0.09	3	1×10^{-11}	1×10^{-10}	5×10^{-11}	0.12	
Sm	50	5	600	1×10^{-11}	1×10^{-10}	5×10^{-11}	0.12	
Eu	50	5	600	1×10^{-11}	1×10^{-10}	5×10^{-11}	0.12	
Ho	50	5	600	1×10^{-11}	1×10^{-10}	5×10^{-11}	0.12	
Pb	2	0.02	300	1×10^{-11}	1×10^{-10}	5×10^{-11}	0.12	
Po	0.1	0.04	0.7	1×10^{-12}	3×10^{-12}	5×10^{-12}	0.06	Anion
Ra	7×10^{-4}	1×10^{-4}	0.005	1×10^{-11}	1×10^{-10}	5×10^{-11}	0.12	
Ac	10	1	200	1×10^{-11}	1×10^{-10}	5×10^{-11}	0.12	
Th	50	10	200	1×10^{-11}	1×10^{-10}	5×10^{-11}	0.12	
Pa	5	0.2	100	1×10^{-11}	1×10^{-10}	5×10^{-11}	0.12	
U	20	0.5	200	1×10^{-11}	1×10^{-10}	5×10^{-11}	0.12	
Np	50	5	500	1×10^{-11}	1×10^{-10}	5×10^{-11}	0.12	
Pu	20	1	300	1×10^{-11}	1×10^{-10}	5×10^{-11}	0.12	
Am	10	1	200	1×10^{-11}	1×10^{-10}	5×10^{-11}	0.12	
Cm	10	1	200	1×10^{-11}	1×10^{-10}	5×10^{-11}	0.12	

Tab. B-16: Probability distribution functions (PDFs) for probabilistic calculations SF/HLW/ ILW; values taken from Nagra (2002b).

For some parameters, correlations between waste types / radionuclides / species (anions, non-anions) have been considered (for details see Nagra 2002c).

SF/HLW Near field	**Parameter values**	
Model parameter	**Reference Case values**	**PDF attributes**
Cladding dissolution rate	3×10^{-5} 1/a	**Lognormal** median = Reference Case value, σ(log) = 0.35 upper truncation = 1.5×10^{-4} a^{-1} (2 σ) lower truncation = 6×10^{-6} a^{-1} (2 σ)
IRF	Tab. B-8 (weighted average)	**Log-uniform** lower cut-off - values for 48 GWd/t_{IHM} PWR fuel (best estimate) upper cut-off - values for 75 GWd/t_{IHM} PWR fuel (Tab. B-17)
SF matrix dissolution rate	Tab. B-10 (weighted average)	**Log-uniform** maximum = reference rate (t) minimum = solubility limited rate (t)
HLW dissolution rate	Tab. B-18	**Triangular** maximum = pessimistic variation values (Tab. B-18) minimum = 0.05 × reference value
Radionuclide solubilities	Tab. B-11	**Discrete** Probability (P) = 0.7 for reference value P = 0.15 for optimistic and pessimistic values
K_d values	Tab. B-14	**Discrete** P = 0.7 for reference value P = 0.15 for optimistic and pessimistic values
Bentonite D_e	Tab. B-14	**Log-normal** median = reference values, σ (log) = 0.3 upper truncation = 2 × reference values (1 σ) lower truncation = 0.1 × reference values (3.3 σ)
ILW Near field	**Parameter values**	
Model parameter	**Reference Case values**	**PDF attributes**
Radionuclide solubilities	Tab. B-13	**Discrete** Probability (P) = 0.7 for reference value P = 0.15 for optimistic and pessimistic values
K_d values	Tab. B-12	**Discrete** P = 0.7 for reference value P = 0.15 for optimistic and pessimistic values

Tab. B-16: (Cont.)

Opalinus Clay	**Parameter values**	
Model parameter	**Reference Case values**	**PDF attributes**
K_d values	Tab. B-15	**Discrete** P = 0.7 for reference value P = 0.15 for optimistic and pessimistic values
Transport path length	40 m	**Uniform** minimum = 40 m maximum = 60 m
D_e	Tab. B-15	**Log-normal** median = reference values, σ (log) = 0.24 upper truncation = 3 × reference values (2 σ) truncation = 0.5 × reference values (1.26 σ)
Darcy velocity	2×10^{-14} m s^{-1}	**Log-normal** median = reference values, σ (log) = 1 upper truncation = 2×10^{-13} m s^{-1} (1 σ) lower truncation = 1×10^{-15} m s^{-1} (1.3 σ)
Transmissivity of hypothetical transmissive discontinuity	-	-

Tab. B-17: IRF values of key radionuclides for BWR and PWR UO^2 fuel and PWR MOX fuel; values taken from Nagra (2002a).

In all cases, the IRF is applied to the radionuclide inventory present in the fuel matrix. In the case of ^{14}C, there is an additional IRF of 20 % assumed for the inventory of the cladding.

Nuclide	**$t_{½}$ [a]**	**IRF Value [%]**			
		BWR UO_2 Fuel (48 GWd/t_{IHM})	**PWR UO_2 Fuel (48 GWd/t_{IHM})**	**PWR UO_2 Fuel (75 GWd/t_{IHM})**	**PWR MOX Fuel (48 GWd/t_{IHM})**
^{3}H	1.23×10^{1}	1	1	1	1
^{10}Be	1.6×10^{6}	10	10	10	10
^{14}C	5.73×10^{3}	10	10	10	10
^{36}Cl	3.0×10^{5}	13	10	25	15
^{79}Se	1.1×10^{6}	9	4	25	15
^{90}Sr	2.86×10^{1}	1	1	1	1
^{99}Tc	2.1×10^{5}	2	2	17	2
^{107}Pd	6.5×10^{6}	2	2	17	2
^{126}Sn	2.3×10^{5}	9	4	25	15
^{129}I	1.57×10^{7}	9	4	25	15
^{135}Cs	2.3×10^{6}	5	4	25	10
^{137}Cs	3.02×10^{1}	5	4	25	10

Tab. B-18: Reference HLW near field parameter values; values taken from Nagra (2002b).

Parameter	Reference value	Variations
Time of canister failure	10^4 a	
Glass corrosion rate		
MW glass (WA-BNF-1)	5.5×10^{-4} kg/(m^2 a)	4.0×10^{-2} kg/(m^2 a)
SON-68 glass (WA-COG-1)	7.3×10^{-5} kg/(m^2 a)	4.0×10^{-2} kg/(m^2 a)
Number of canisters n_{COG} n_{BNFL}	 460 270	
Length of glass blocks, h	752 m (1.03 m for each block, 730 blocks)	
Initial diameter of glass blocks, d_0	0.43 m	
Glass density	2750 kg/m^3	
Factor of glass surface area increase due to fracturing	15	
Volume for dissolution, V_R (thickness, d*, of reservoir)	d = 2.5 cm 24.6 m^3 (0.037 m^3 for each block)	
Canister radius	0.47 m	
Inner bentonite radius	0.47 m	
Outer bentonite radius	1.15 m	
Bentonite porosity	0.36	
Bentonite solid density	2760 kg/m^3	

* d represents a 2.5 cm thick annular region surrounding each glass block.

Tab. B-19: Biosphere dose conversion factors (BDCFs); values taken from Nagra (2002a).

The BDCF for a given radionuclide is the ratio of the corresponding steady-state annual dose [Sv/a] to the input value of 1 Bq/a. For each radionuclide, a constant flux of 1 Bq/a is input into the transient compartment model, with the Reference Case conceptual assumptions and parameters, and the model is run until a steady state is reached.

Nuclide	Biosphere dose conversion factor [Sv/Bq]
^{3}H	1.68×10^{-16}
^{10}Be	4.82×10^{-16}
^{14}C	4.48×10^{-15}
^{36}Cl	9.86×10^{-15}
^{41}Ca	4.33×10^{-16}
^{59}Ni	1.62×10^{-16}
^{60}Co	3.41×10^{-17}
^{63}Ni	6.18×10^{-18}
^{79}Se	1.89×10^{-14}
^{90}Sr	4.00×10^{-15}
^{93}Mo	3.74×10^{-15}
^{93m}Nb	1.42×10^{-18}
^{93}Zr	9.41×10^{-15}
^{94}Nb	2.00×10^{-13}
^{99}Tc	6.75×10^{-14}
^{107}Pd	9.96×10^{-17}
^{108m}Ag	1.20×10^{-14}
^{121m}Sn	2.07×10^{-17}
^{126}Sn	4.37×10^{-14}
^{129}I	2.48×10^{-13}
^{135}Cs	3.64×10^{-14}
^{137}Cs	1.94×10^{-16}
^{151}Sm	7.65×10^{-19}
^{154}Eu	4.34×10^{-18}
^{166m}Ho	1.72×10^{-14}
^{210}Pb	3.82×10^{-15}
^{210}Po	9.12×10^{-18}

Nuclide	Biosphere dose conversion factor [Sv/Bq]
^{226}Ra	4.20×10^{-13}
^{227}Ac	1.49×10^{-15}
^{228}Ra	8.03×10^{-16}
^{228}Th	4.54×10^{-18}
^{229}Th	8.10×10^{-14}
^{230}Th	5.14×10^{-12}
^{231}Pa	1.72×10^{-11}
^{232}Th	4.60×10^{-12}
^{232}U	4.78×10^{-15}
^{233}U	8.14×10^{-14}
^{234}U	2.56×10^{-13}
^{235}U	2.84×10^{-12}
^{236}U	3.52×10^{-14}
^{237}Np	3.03×10^{-13}
^{238}Pu	3.52×10^{-16}
^{238}U	3.98×10^{-14}
^{239}Pu	5.23×10^{-14}
^{240}Pu	2.13×10^{-14}
^{241}Am	1.24×10^{-15}
^{241}Pu	4.23×10^{-17}
^{242m}Am	4.96×10^{-16}
^{242}Pu	9.04×10^{-14}
^{243}Am	3.56×10^{-14}
^{243}Cm	1.34×10^{-16}
^{244}Cm	9.38×10^{-17}
^{245}Cm	5.70×10^{-14}
^{246}Cm	1.77×10^{-14}

Appendix C: L/ILW repository input parameters

Tab. C-1: Reference inventories for L/ILW; values taken from Nagra (2008a).

Radionuclide	Inventory [Bq]
^{10}Be	1.4×10^{9}
$^{14}C_{inorg}$	1.1×10^{13}
$^{14}C_{org}$	4.3×10^{14}
^{36}Cl	5.2×10^{12}
^{40}K	1.6×10^{9}
^{59}Ni	1.2×10^{15}
^{60}Co	1.5×10^{17}
^{63}Ni	2.3×10^{17}
^{79}Se	2.1×10^{11}
^{90}Sr	1.8×10^{13}
^{93}Mo	1.8×10^{13}
^{94}Nb	7.0×10^{12}
^{108m}Ag	7.5×10^{12}
^{126}Sn	4.2×10^{10}
^{129}I	1.6×10^{8}
^{137}Cs	1.6×10^{14}
^{210}Pb	5.6×10^{10}
^{210}Po	5.5×10^{10}
^{226}Ra	1.0×10^{11}
^{227}Ac	1.4×10^{7}
^{228}Ra	6.0×10^{8}
^{228}Th	7.2×10^{9}
^{229}Th	1.3×10^{7}

Radionuclide	Inventory [Bq]
^{230}Th	1.2×10^{7}
^{231}Pa	8.3×10^{6}
^{232}Th	6.5×10^{8}
^{232}U	6.5×10^{9}
^{233}U	4.0×10^{9}
^{234}U	1.9×10^{10}
^{235}U	1.2×10^{9}
^{236}U	4.3×10^{8}
^{237}Np	2.5×10^{7}
^{238}Pu	1.7×10^{12}
^{238}U	1.1×10^{10}
^{239}Pu	4.9×10^{11}
^{240}Pu	3.2×10^{11}
^{241}Am	2.3×10^{12}
^{241}Pu	2.3×10^{13}
^{242m}Am	1.1×10^{9}
^{242}Pu	1.4×10^{9}
^{243}Am	2.6×10^{10}
^{243}Cm	5.1×10^{9}
^{244}Cm	2.5×10^{12}
^{245}Cm	6.4×10^{8}
^{246}Cm	7.3×10^{9}

Tab. C-2: L/ILW near field data; values taken from Nagra (2008a).

Parameter	**Reference value**
Length of emplacement tunnels	Waste group L/ILW-1: 800 m (4 tunnels with 200 m length each) Waste group L/ILW-2: 600 m (3 tunnels with 200 m length each)
Cross-sectional area tunnel	110 m^2
Backfill	Cement
Porosity	0.2
Sorption-relevant amount of solid phase	350 kg/m^3
Hydraulic Conductivity	10^{-6} m/s
Dispersion length (longitudinal / transversal)	2 / 0.2 m
Effective diffusion coefficient	2×10^{-10} m^2/s

Tab. C-3: Sorption values (K_d) for waste group 1 and 2 in the L/ILW near field; values taken from Nagra (2008a).

Values for non-degraded and degraded cement.

Element	Waste group 1 K_d [m^3/kg]		Waste group 2 K_d [m^3/kg]	
	Non-degraded	degraded	Non-degraded	degraded
H	1×10^{-4}	0	1×10^{-4}	0
Be	0	0	0	0
C_{inorg}	0.4	0.001	0.4	0.001
C_{org}	0	0	0	0
Cl	0.005	0	0.005	0
K	0	0	0	0
Co	0.01	0.002	0	0.002
Ni	1	5×10^{-4}	0	5×10^{-4}
Se	0.03	0	0.03	0
Sr	0.001	5×10^{-5}	0.001	5×10^{-5}
Zr	10	0.7	1	0.7
Nb	1	0	1	0
Mo	0	0	0	0
Tc	0.001	0	0.001	0
Ag	0	0	0	0
Sn	10	0	1	0
I	0.001	0	0.001	0
Cs	5×10^{-4}	0	5×10^{-4}	0
Sm	20	1	2	1
Eu	20	1	2	1
Pb	0.5	0.1	0.05	0.1
Po	0	0	0	0
Ra	0.05	5×10^{-5}	0.05	5×10^{-5}
Ac	20	1	2	1
Th	5	0.7	0.5	0.7
Pa	0.1	0.04	0.1	0.04
U	2	0.2	2	0.2
Np	5	0.1	0.5	0.1
Pu	5	0.1	0.5	0.1
Am	20	1	2	1
Cm	20	1	2	1

Tab. C-4: Time-dependend life time and degradation of the L/ILW cementitious near field; values taken from Nagra (2008d).

Water flow *q* in the host rock [m/s]	**Waste group 1**			**Waste group 2**		
	Non-degraded	Linear Transition	Degraded	Non-degraded	Linear Transition	Degraded
$< 1 \times 10^{-12}$	$t < \infty$	-	-	$t < \infty$	-	-
1×10^{-12}	$t < 6 \times 10^{6}$ a	6×10^{6} a $\leq t \leq 1.8 \times 10^{7}$ a	$t > 1.8 \times 10^{7}$ a	-	0 a $\leq t \leq 1.2 \times 10^{7}$ a	$t > 1.2 \times 10^{7}$ a
1×10^{-11}	$t < 6 \times 10^{5}$ a	6×10^{5} a $\leq t \leq 1.8 \times 10^{6}$ a	$t > 1.8 \times 10^{6}$ a	-	0 a $\leq t \leq 1.2 \times 10^{6}$ a	$t > 1.2 \times 10^{6}$ a

Tab. C-5: Probability distribution functions (PDFs) for probabilistic calculations L/ILW.

Host rock	**Parameter values**	
Model parameter	**Reference Case values**	**PDF attributes**
K_d values	Tab. B-15	**Discrete** P = 0.7 for reference value P = 0.15 for optimistic and pessimistic values
Transport path length	40 m	**Uniform** minimum = 40 m maximum = 100 m
D_e	Tab. B-15	**Log-normal** median = reference values, σ (log) = 0.24 upper truncation = 3 × reference values (2 σ) truncation = 0.5 × reference values (1.26 σ)
Darcy velocity	1×10^{-13} m s^{-1}	**Log-normal** median = reference values, σ (log) = 1 upper truncation = 1×10^{-11} m s^{-1} (1 σ) lower truncation = 1×10^{-15} m s^{-1} (1 σ)

Appendix D: Sharing experience

Presentations of the final PAMINA meeting, September 28-30, 2009, Hohenkammer, Germany, Session VI – Probabilistic safety assessment:

- Development of a new PSA approach – Sharing experience: Jürg Schneider, Nagra
- Pilot study on PSA: Gerhard Mayer, AF Colenco Ltd.

Contents

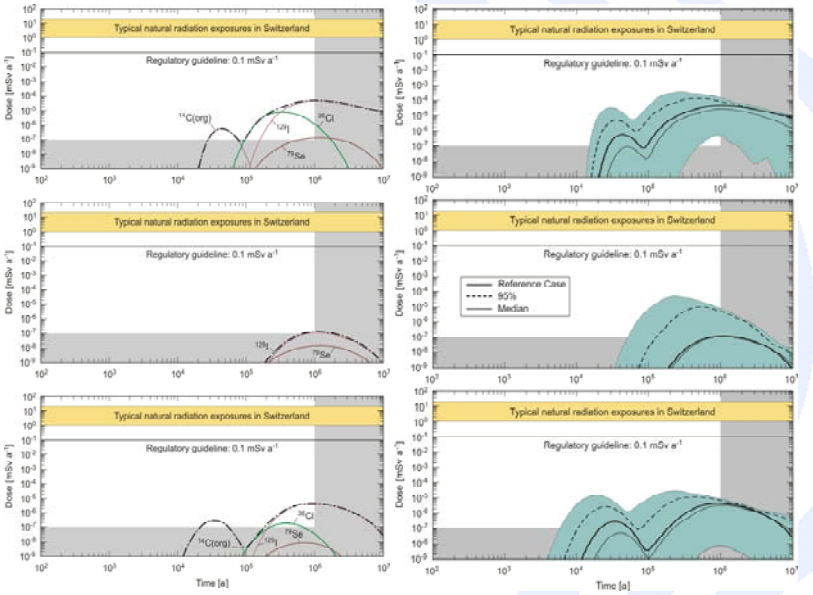
- Introduction
- Methodology
- Requirements for the new tool
- Code development
- Status & outlook
- Conclusions

Introduction

Starting point: Safety Case for Project Opalinus Clay (Entsorgungsnachweis) → Nagra reports NTB 02-05, 02-06, 02-23 (www.nagra.ch)

- Demonstration of disposal feasibility for SF, HLW and ILW
- Based on a site in northern Switzerland (Zürcher Weinland)
- Approach to assess radionuclide release and transport:
  A combination of deterministic and probabilistic analyses
- Deterministic analyses
  - spectrum of analyses results in spectrum of consequences
  - results easy to understand and easy to explain (esp. to non-specialists)
  - but: unfavourable combinations of parameter values may be overlooked
- Probabilistic analyses
  - consequences take into account combined effects of uncertainties
  - provide assurance that no unfavourable combinations of parameter values exist that can compromise safety

Deterministic and Probabilistic Analyses



SF

HLW

ILW

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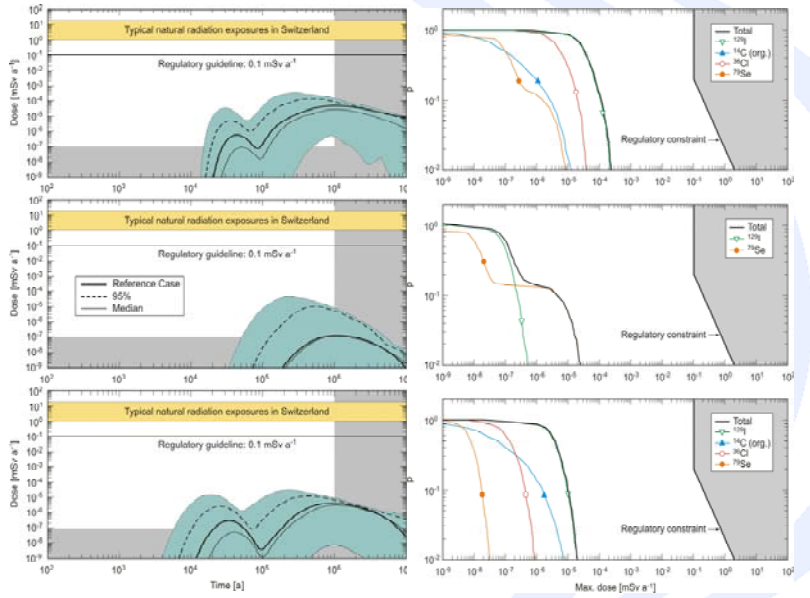
PSA (distributed evolution of dose, CCDFs)



SF

HLW

ILW

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Introduction (continued)

- After Project Opalinus Clay (Entsorgungsnachweis): Decision to strengthen PSA approach
  → Start of a PSA development project in 2005
- Phase 1: Pilot Study (see next presentation)
  - concluded in July 2006
  - limitations of approach used in Pilot Study: simultaneous and parallel modelling of all relevant phenomena is not possible
- Phase 2: Development of a probabilistic approach considering all potentially relevant phenomena (esp. role of gas)
  - start in 2006
  - Nagra participation in PAMINA with this project under the motto "sharing experience"
  - key (starting) point: establish a process to derive a comprehensive list of relevant phenomena to be included in PSA tool
  - then: develop and apply PSA tool

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Methodology

- The steps
  - how to develop the PSA tool
  - how to manage & run the PSA tool
- Philosophy
  - ensure that the broad range of uncertainties is adequately captured
    → get the scientists directly involved in a clearly defined process
  - establish such a process to derive a comprehensive list of relevant phenomena to be included in PSA tool → list of "accepted FEPs" for PSA
  - develop a tool capable of simultaneously modelling all accepted FEPs and their interactions (ambitious task)
  - recognise from the start that such a tool may (initially) not run sufficiently fast for large numbers of probabilistic calculations
  - but: if that should turn out to be the case, then the tool could be successively simplified until it runs fast enough for PSA calculations
  - advantages of such an approach
    - "automatic" benchmarks on the way from "more detailed" to "more simple"
    - the effects of simplifications can be monitored
    - already running the tool deterministically will yield insights into the effects of simultaneous consideration of all relevant FEPs

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Requirements for the new tool (1)

Development of a comprehensive list of relevant FEPs to be included

- Establishment of a working group for this task (August 2006)
- Specialists included experts in safety analysis, radionuclide transport modelling, gas transport modelling, waste characteristics, geochemistry, geosciences, etc.
- If an identified FEP required special attention, new sub-groups with additional experts were formed to address this FEP, in some cases supported by complementary process modelling (example: FEPs No. 1.5.4: High-pH plume: sealing effect in host rock; No. 1.5.11: High-pH plume: tunnel backfill sealing effect)
- 10 expert meetings were held overall (documented in internal notes)
- Results documented in FEP Screening Report NAB 07-38 (PAMINA RTDC2 Milestone Report M2.2.E.2)

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Requirements for the new tool (2)

Development of FEP list (continued)

- Step-wise procedure
  - development of a broad list of potentially safety-relevant FEPs → 86 potentially safety-relevant FEPs
  - discussion of the potentially safety-relevant FEPs with respect to
    - relevance with regard to Swiss repository types & potential host rocks
    - process understanding
    - evaluation of the effect of the FEP
  - judgement whether or not an individual FEP should be included in the list of accepted FEPs → 52 accepted FEPs to be included in the new tool

Other requirements

- For each module in the suite of codes three types of requirements were defined before the start of development work
  - functional requirements (related to the accepted FEPs)
  - interface requirements (related to data transfer between modules)
  - performance requirements (related to module performance)

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Code development: Overview

- Software architecture ▷
- Development needs (based on a review of the capabilities of existing codes and the requirements defined in the previous step)
  - TREETOOL: developed parallel to Phase 1 for a simplified example PSA tool
  - GOLDSIM probabilistic driver: operational & tested for simplified models
  - IRRC: deterministic "engine" of the new PSA tool (large effort required)
    - STMAN-TD: further development of existing version (time-dependent flow boundary conditions → small effort required)
    - PICNIC-TD: new development needed (existing version cannot handle time-dependent flow due to solver type used → medium effort required)
    - GAS MODEL (transport of volatile nuclides in the gas phase): minor development needs (simplified treatment)
    - IFC: major development effort required
    - Input Data Converters: significant development effort required
    - Interfaces & integration of modules: development effort required

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Integrated Flow Code IFC

- Development of IFC based on TOUGH2
- Time-dependent two-phase flow in the near field and geosphere of a gas-generating nuclear waste repository system for SF / HLW / ILW located in a claystone host rock (Opalinus Clay)
- Provides water and gas flow fields as input to subsequent radionuclide transport calculations

1. Numerical code
   - modification of the multiphase, multicomponent simulator TOUGH2
   - code modifications: (i) implementation of "accepted FEPs"; (ii) removal of processes and features that are not needed (speed!)
2. Model repository system (simplified representation of the repository) → computational mesh
   - emplacement tunnels for SF / HLW / ILW
   - engineered barriers (backfill, seals, plugs, etc.) & other underground structures
   - geological structures (host rock, EDZ, confining units, local aquifers)

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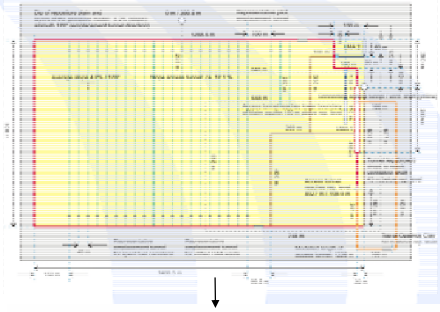
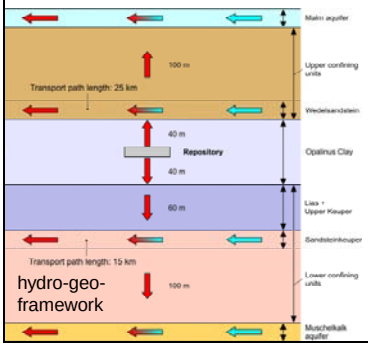
IFC (continued)

Repository layout

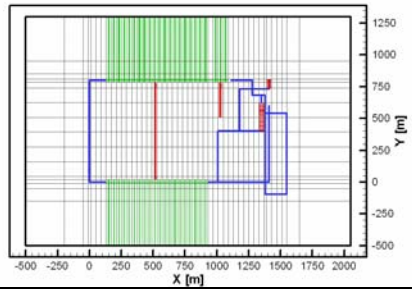
Equivalent conceptual repository model





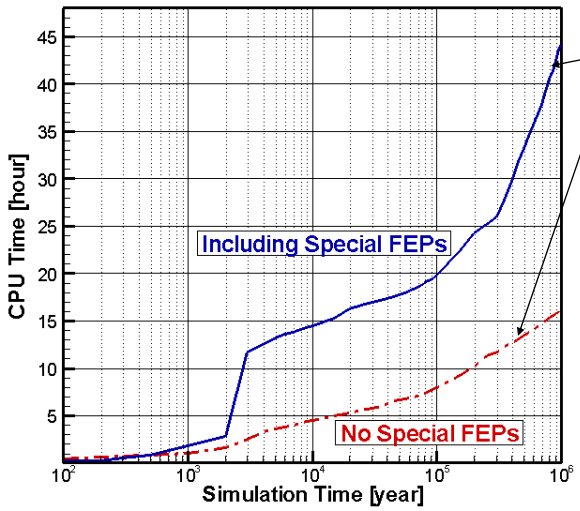
hydro-geo-framework

IFC model (computational mesh)



IFC (continued)

CPU time as a function of simulation time



all FEPs included

some FEPs excluded:

- pathway dilation
- EDZ self-sealing
- tunnel convergence
- uplift
- geochemical sealing

CPU-time-intensive tasks:

- simulating strong changes at early times with initial expansion of 2-phase zone
- resolving nonlinearities and counteracting effects (early-time pressure increase combined with tunnel convergence; late-time transient effects due to uplift)

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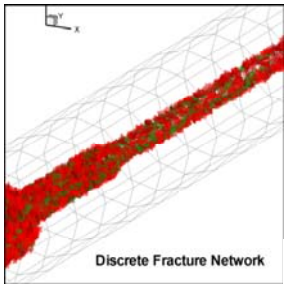
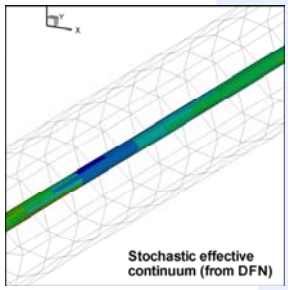
EDZ Converter (1)

Successive model abstraction

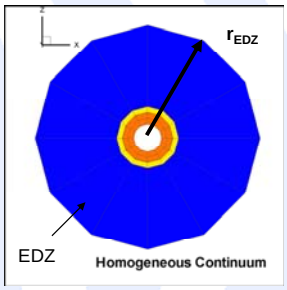
The model to our best geoscientific understanding



Heterogeneous continuum porous medium model ("CPM")



The model suitable for PA calculations ("sim.")



Combined gas/water flow

Simulate pressure & flow with the CPM model – fit simplified homogeneous model → effective parameters (r_{EDZ} , k_{EDZ}, rel. perm., cap. pr., ...)

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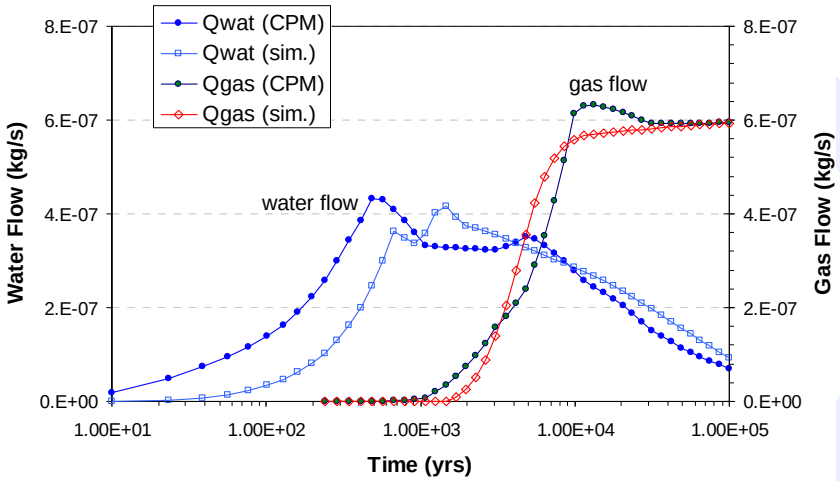
EDZ Converter (2)



→ **simulated responses (pressure and gas / water flow) from the CPM model can be used to calibrate effective parameters for a simplified homogeneous model**

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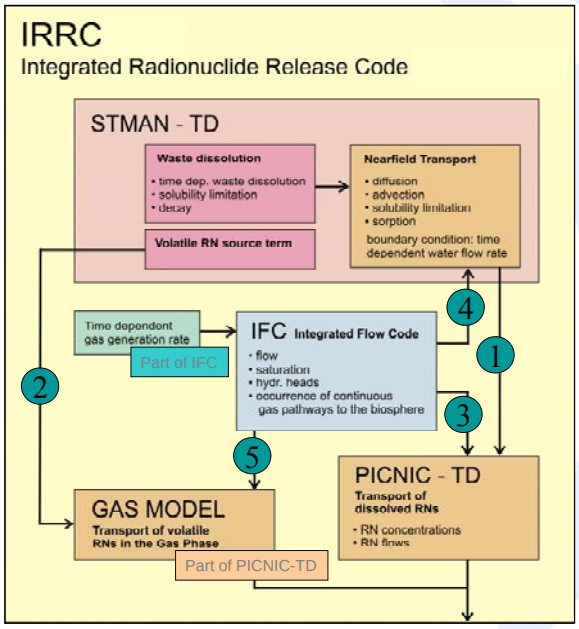
Integration of modules: IRRC



Codes

STMAN-TD
PICNIC-TD (with Gas Model)
IFC

Linkages

1 STMAN to PICNIC
2 STMAN to Gas Model
3 IFC to PICNIC
4 IFC to STMAN
5 IFC to Gas Model

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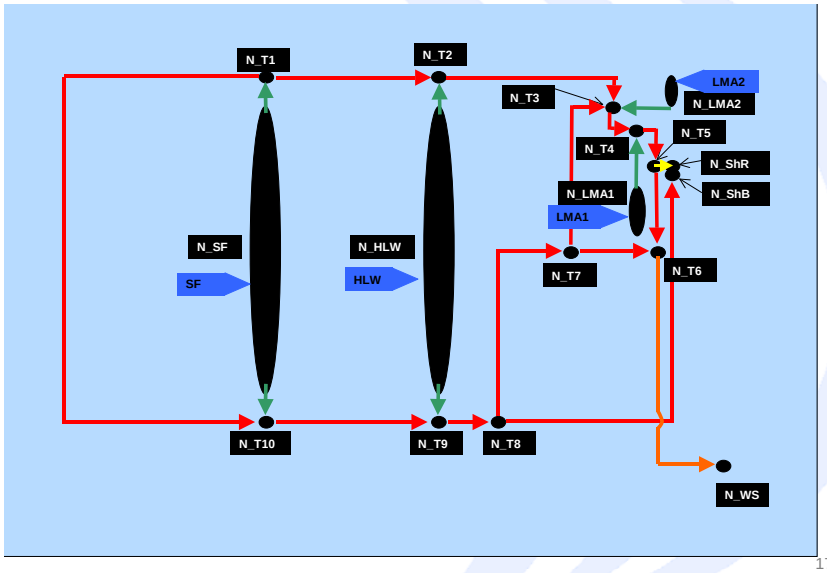
IFC–PICNIC linkage network (h)

h: horizontal plane



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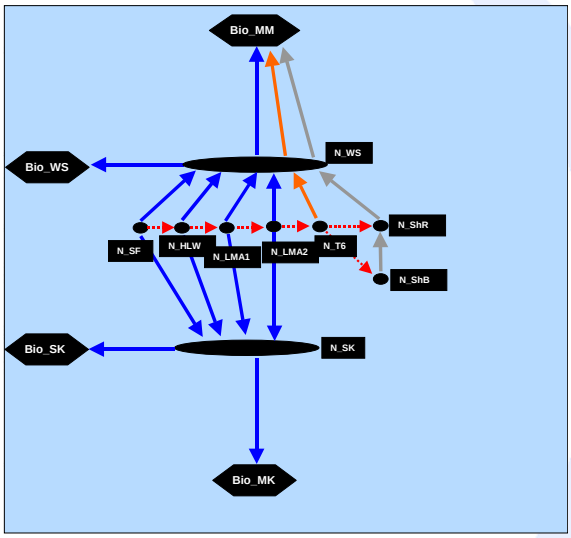
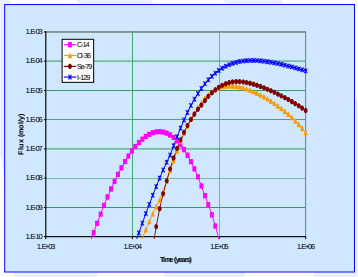
IFC–PICNIC linkage network (v)

v: vertical plane



Results (example: Bio_WS)



Case with 36 legs, 39 nuclides & full IFC flow field (previously calculated): 40 Min.
no MD from tunnels: 8 Min.
no flow in tunnels: ~ 3 Min.
(but results very similar)

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Status & outlook

- Status: IRRC is up and running, but ...
  - maximum version with all accepted FEPs included is relatively slow
  - max. CPU time needed for IFC (~ 45 h for 1 Ma with all accepted FEPs)
  - rest of IRRC calculations ~ 40 Min. with all radionuclide processes
  - a number of preliminary functionality tests completed successfully
  - on-going project
- Outlook
  - gain further experience with running full IRRC
  - successively reduce number of FEPs included and continuously monitor effect on calculated releases and on CPU time needed
  - build full PSA tool (GOLDSIM, TREETOOL)
  - run and test PSA tool
  - for operational applications
    - adapt mesh (repository design has been modified in the meantime)
    - implement expert elicitation process to obtain required input (scenarios, conceptual models, data (PDFs))
  - in parallel: develop simple, modular PSA tools using the GOLDSIM probabilistic driver and established radionuclide release & transport codes for SF / HLW / ILW / L/ILW for first applications (on-going)

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Conclusions

- Development of a fully probabilistic approach started in 2006 is well under way (on-going project)
- Development of FEP list and IRRC was more difficult & time consuming than originally thought (involvement of large team of experts from many disciplines; recruited as required by progress of project)
- Stand-alone IRRC
  - unique tool fully incorporating 52 “accepted FEPs” derived in a systematic manner
  - very useful tool “in its own right”
  - excellent basis for further development (key part of “full” PSA tool):
    systematic reduction of no. of FEPs included while monitoring effects on
    - calculated releases
    - CPU time needed

    benchmarks obtained “for free” (“maximum version” → “reduced version”)
- New versions of NF code and geosphere transport code developed “on the way” (STMAN-TD, PICNIC-TD) for time-dependent flow
- Simplified modular PSA tools developed in parallel for first applications

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PAMINA

Thank you!

PAMINA Final Workshop, September 28-30, 2009
Hohenkammer, Germany

PAMINA

Probabilistic Safety Assessment

Pilot Study on PSA

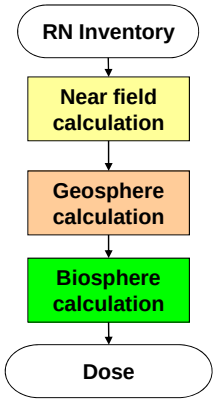
Gerhard Mayer, AF-Colenco

Contents

- Introduction
- Tools for deterministic RN calculation
- Probabilistic tool: @RISK
- Application to High Level Waste Repository
  - Reference Conceptualisation
  - RN release affected by ramp / shaft
- Conclusions

Report NAB 07-09 (in German) available at NAGRA

Toolbox for deterministic RN release calculations



- STMAN
  - Release of dissolved RN from near field
- PICNIC
  - Transport of dissolved RN through geosphere
- TAME
  - Biosphere compartment model

Toolbox for deterministic RN release calculations

- Each Tool is well tested
- Combination of tools gives high flexibility
- Adjustable level of detail
  - Simplified ⇔ Fast
  - Detailed ⇔ Slow
- Toolbox does not cope with all identified FEPs
- (Toolbox has been extended)

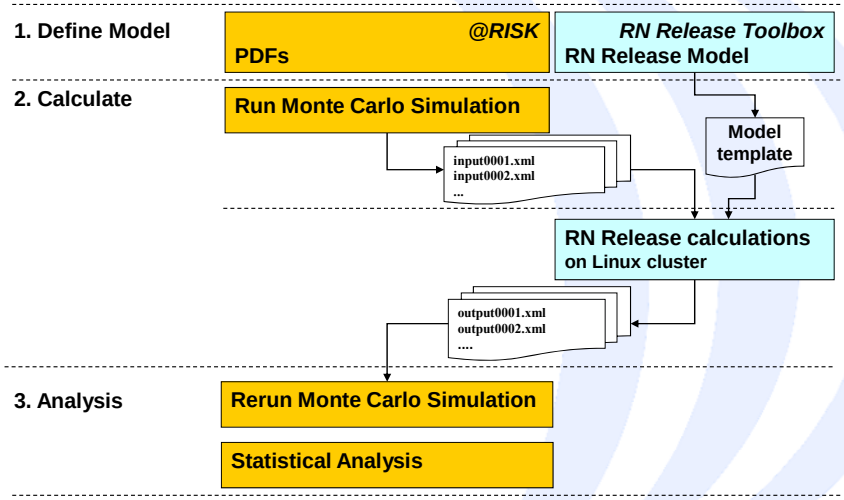
Requirements for probabilistic tool

- Definition of probabilistic distribution functions
- Generation of realizations
- ~~Calculation of RN release~~ ⇐ Toolbox for RN release calculations
- Statistical analysis of results

@RISK

- Commercial Excel add-in
- Definition of Probabilistic Distribution Functions
- Sampling
  - ☑ Monte Carlo
  - ☑ Latin hypercube
- Statistical analysis
  - ☐ Time series
  - ☑ Convergence Monitor
- Interfacing with Toolbox for RN release calculations by reading and writing XML-files using VBA

Workflow



Application: Max. Dose from a High Level Waste Repository in Opalinus Clay

- Processes considered
  - Time dependent release from waste packages
  - Transport of dissolved RN due to advection, dispersion/diffusion
  - Sorption
  - Solubility limitation
- Not considered here:
  - Release of volatile RN
  - Effects of gas generation
  - Coupled processes (HM, THM, THMC…)

Application: Max. Dose from a High Level Waste Repository in Opalinus Clay (II)

Probabilistic parameters of near field

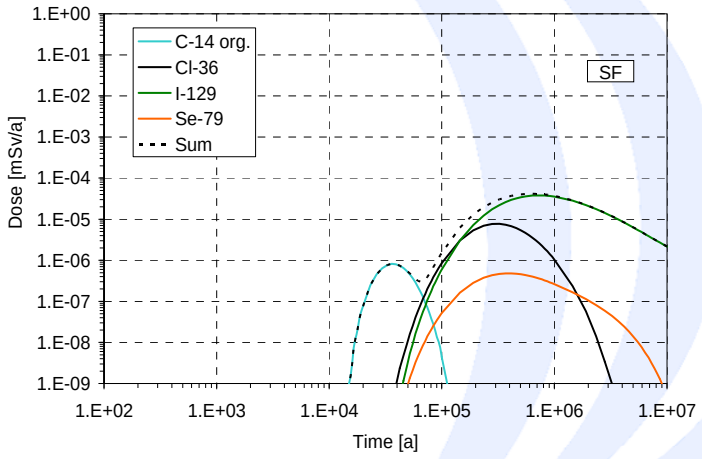
- Spent Fuel
  - Instant release fraction (IRF) and matrix dissolution rate
  - Diffusion Coefficients in bentonite buffer
  - Kd-Values in bentonite buffer
  - Solubility limits
- Vitrified high level waste
  - Glass dissolution rate
  - Diffusion Coefficients in bentonite buffer
  - Kd-Values in bentonite buffer
  - Solubility limits
- Intermediate level waste
  - Kd-Values in cemented waste
  - Solubility limits

Probabilistic parameters of geosphere

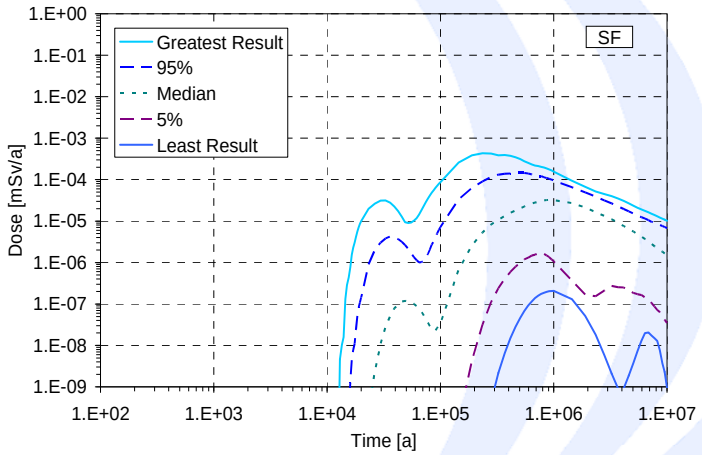
- Darcy velocity in host rock
- Diffusion coefficients
- Kd-Values
- Transport path length

In total: 176 Parameters

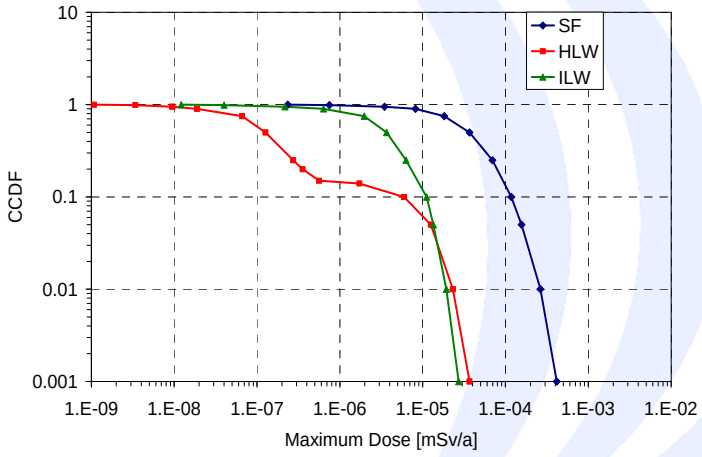
SF Reference Case (Deterministic)



SF, 1000 samples

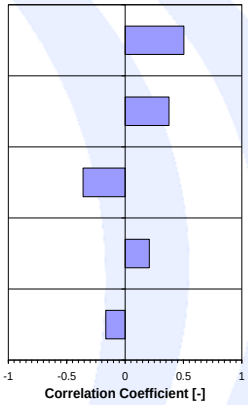


SF, HLW, ILW: CCDF



Correlation of parameters with max. total dose

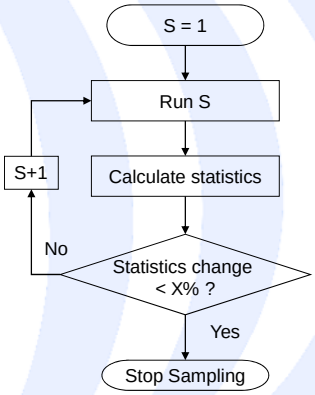
1. Darcy velocity in host rock
2. Instant release fraction of Iodine
3. Sorption coefficient of Iodine in host rock
4. Diffusion coefficient in host rock
5. Transport path length in host rock



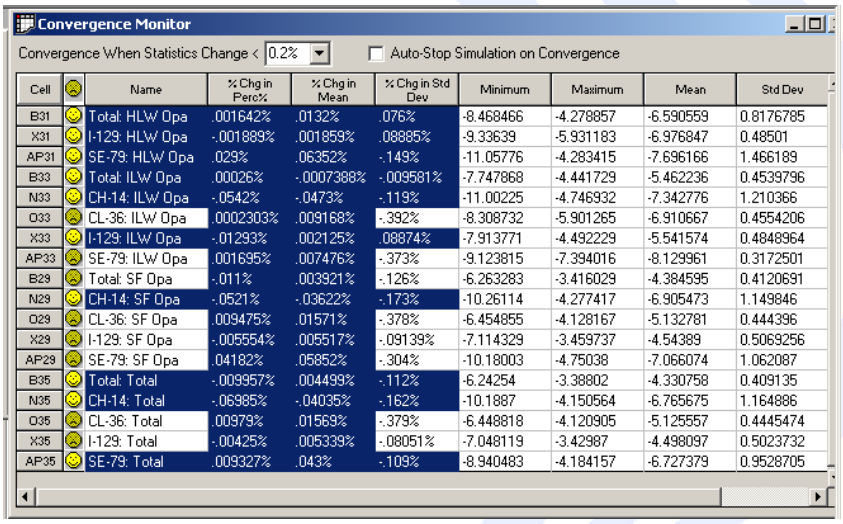
- **176 parameters have been diced**
- **About 5 are sensitive**

10, 100, 1000, 10000, … How many samples are required?

- Approach:
  Stop sampling when
  Statistics change < X %
- Statistics used by @RISK
  - Percentile
    - 0-5%, 5% -10%, …,95%-100%
  - Mean
  - Standard deviation of mean



Convergence Monitor

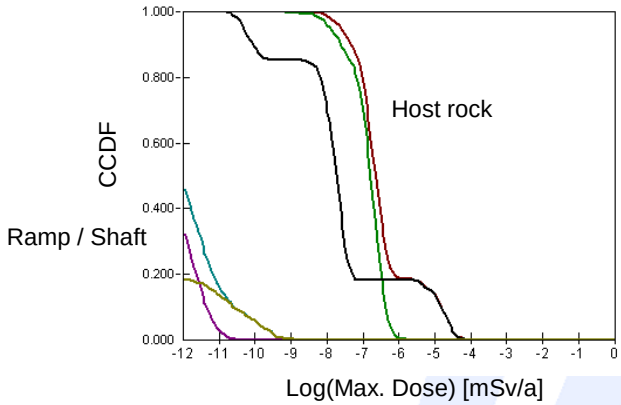


Cell	Name	% Chg in Perc%	% Chg in Mean	% Chg in Std Dev	Minimum	Maximum	Mean	Std Dev
B31	Total: HLW Opa	.001642%	.0132%	.076%	-8.468466	-4.278857	-6.590559	0.8176785
X31	I-129: HLW Opa	-.001889%	.001859%	.08885%	-9.33639	-5.931183	-6.976847	0.48501
AP31	SE-79: HLW Opa	.029%	.06352%	-.149%	-11.05776	-4.283415	-7.696166	1.466189
B33	Total: ILW Opa	.00026%	-.0007388%	-.009581%	-7.747868	-4.441729	-5.462236	0.4539796
N33	CH-14: ILW Opa	-.0542%	-.0473%	-.119%	-11.00225	-4.746932	-7.342776	1.210366
O33	CL-36: ILW Opa	.0002303%	.009168%	-.392%	-8.308732	-5.901265	-6.910667	0.4554206
X33	I-129: ILW Opa	-.01293%	.002125%	.08874%	-7.913771	-4.492229	-5.541574	0.4848964
AP33	SE-79: ILW Opa	.001695%	.007476%	-.373%	-9.123815	-7.394016	-8.129961	0.3172501
B29	Total: SF Opa	-.011%	.003921%	-.126%	-6.263283	-3.416029	-4.384595	0.4120691
N29	CH-14: SF Opa	-.0521%	-.03622%	-.173%	-10.26114	-4.277417	-6.905473	1.149846
O29	CL-36: SF Opa	.009475%	.01571%	-.378%	-6.454855	-4.128167	-5.132781	0.444396
X29	I-129: SF Opa	-.005554%	.005517%	-.09139%	-7.114329	-3.459737	-4.54389	0.5069256
AP29	SE-79: SF Opa	.04182%	.05852%	-.304%	-10.18003	-4.75038	-7.066074	1.062087
B35	Total: Total	-.009957%	.004499%	-.112%	-6.24254	-3.38802	-4.330758	0.409135
N35	CH-14: Total	-.06985%	-.04035%	-.162%	-10.1887	-4.150564	-6.765675	1.164886
O35	CL-36: Total	.00979%	.01569%	-.379%	-6.448818	-4.120905	-5.125557	0.4445474
X35	I-129: Total	-.00425%	.005339%	-.08051%	-7.048119	-3.42987	-4.498097	0.5023732
AP35	SE-79: Total	.009327%	.043%	-.109%	-8.940483	-4.184157	-6.727379	0.9528705

How many samples are required?

Convergence criterion	Number of samples	Mean Maximum Dose [mSv/a]
14 %	100	$4.14 \cdot 10^{-5}$
2 %	220	$4.75 \cdot 10^{-5}$
1 %	370	$4.74 \cdot 10^{-5}$
0.5 %	660	$4.68 \cdot 10^{-5}$
0.4 %	1000	$4.68 \cdot 10^{-5}$

RN release affected by ramp / shaft



- Dose contribution from pathway ramp / shaft is negligible

How long does it take?

- One sample:
  - 5 x Near field -> 5 minutes
  - 3 x Geosphere -> 3 minutes
  - 3 x Biosphere << 1 minute

  Total: 7-8 minutes / sample

- Using cluster with 10 Quad Core CPUs
  Total: 3 hours for 1000 samples

Conclusions

- Probabilistic Safety Analysis gives valuable insight in system behavior
- Maximum Dose of the investigated repository system affected by a few parameters only (consistent with experience from deterministic calculations)
- Calculation time for a probabilistic performance analysis is fair

- Extension of Toolbox for RN release calculations required to cope with all identified FEPs

- @RISK can be used for Monte Carlo Simulations
- The functionality provided by @RISK for stochastic analysis is limited