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The Use of Numerical Models in Support of Site Characterization and Performance Assessment Studies of Geological Repositories

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THE USE OF NUMERICAL MODELS IN SUPPORT OF SITE CHARACTERIZATION AND PERFORMANCE ASSESSMENT STUDIES OF GEOLOGICAL REPOSITORIES

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THE USE OF NUMERICAL MODELS IN SUPPORT OF SITE CHARACTERIZATION AND PERFORMANCE ASSESSMENT STUDIES OF GEOLOGICAL REPOSITORIES

RESULTS OF AN IAEA COORDINATED RESEARCH PROJECT 2005–2010

INTERNATIONAL ATOMIC ENERGY AGENCY
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FOREWORD

The siting, development and operation of waste disposal facilities, and the related safety issues, have been described in many IAEA publications. The safe management and disposal of radioactive waste from the nuclear fuel cycle remains a necessary condition for future development of nuclear energy. In particular, the disposal of high level waste and spent nuclear fuel in geological repositories, despite having been studied worldwide over the past several decades, still requires full scale demonstration through safe implementation, as planned at the national level in Finland and Sweden by 2020 and 2023, respectively, and in France by 2025. Safety assessment techniques are currently applicable to potential facility location and development through a quite large range of approaches and methodologies.

By implementing research activities through coordinated research projects (CRPs), the IAEA enables research institutes in both developing and developed Member States to collaborate on research topics of common interest. In response to requests by several Member States in different networks and platforms dealing with waste disposal, in 2005 a CRP on The Use of Numerical Models in Support of Site Characterization and Performance Assessment Studies of Geological Repositories was proposed and developed to transfer modelling expertise and numerical simulation technology to countries needing them for their national nuclear waste management programmes.

All Member States involved in this CRP have acquired the scientific basis for, and expertise in, the site characterization process, including test design, data analysis, model calibration, model validation, predictive modelling, sensitivity analysis and uncertainty propagation analysis. This expertise is documented in this publication, in which numerical modelling is used to address the pertinent issue of site characterization and its impact on safety, using data and information from a potential repository site.

The IAEA gratefully acknowledges the contributions of the CRP participants and consultants to the drafting and review of this final report. Special thanks are due to S. Finsterle (USA) for his role in coordinating discussions during the research coordination meetings and for his contributions to drafting and finalizing this report. The IAEA officers responsible for this publication were B. Neerdael and S. Hossain of the Division of Nuclear Fuel Cycle and Waste Management.

CONTENTS

SUMMARY

This CRP, which began in 2005 and was completed in 2010, has the overall purpose to transfer modelling expertise and numerical simulation technology to countries needing them for their national nuclear waste management programmes. Basic activities as part of this CRP consisted of (1) demonstrating the use of modelling strategies to address relevant issues using site-specific data (if available), (2), gain insights in the reliability and uncertainty of numerical model predictions, and (3) improving the modelling capabilities at institutions in the participating Member States.

Five Research Contracts from *Brazil (BRA)*, *China (CPR)*, *Lithuania (LIT)*, *Romania (ROM)* and *Ukraine (UKR)* and two Research Agreements from *India (IND)* and *the Republic of Korea (ROK)* were signed after a merit review of the proposals submitted by prospective participants of this CRP. Moreover, the services of three Scientific Coordinators were secured from *Belgium (BEL), UK* and *USA*. Research activities were coordinated by IAEA and supporting Member States at three Research Coordination Meetings (RCMs) held in Beijing, China, in September 2006, in Daejon, Republic of Korea, in May 2008, and in Kaunas, Lithuania, in November 2009. Progress was evaluated at the RCMs and monitored through review of various interim reports and deliverables.

The general and specific objectives of this CRP are challenging in that they involve the use of advanced simulation technologies to address a wide range of questions related to site characterization and performance assessment for a variety of country-specific waste disposal concepts, waste inventories, and geological formations. The interests expressed in the initial proposal by each selected participating Member State reflected the respective repository system and host formation, specific issues of concern, and available software. The submitted CRP proposals can be categorized as follows:

(1) *Capability development* (specifically studies supporting code selection and development of specific modelling capabilities): CPR, ROM, ROK and IND;
(2) *Code application* (specifically radionuclide transport studies for site selection): UKR, LIT;
(3) *Theoretical studies* (specifically related to TSPA): BRA, CPR, ROK.

Based on these differences and common interests, test cases and comparative studies were identified during the first RCM to arrive at a coordinated and collaborative research programme. In particular, two groups were formed: Group A focused on process modelling issues, whereas Group B examined alternative Total System Performance Assessment (TSPA) methodologies, one based on probabilistic and the other a possibilistic (fuzzy logic-based) approach. The second RCM further evaluated the accomplishments and identified gaps that needed to be filled in order to complete a meaningful comparative analysis. Detailed recommendations and assignments were made, with results expected to be included in country-specific contract reports and two group-specific synthesis reports, which document the work conducted during Phase I (year 1-3) of the CRP. Recommendations made at the end of Phase I provided the basis for the planning of Phase II (Years 4 and 5). It was found that not sufficient information was present (or likely to become available in a timely manner) to continue the investigation of the possibilistic TSPA approach analysed by BRA. Consequently, the contract with BRA was not renewed for Phase II, requiring an adjustment of the comparative work conducted in Group B and its interaction with Group A. This readjustment and the definition of work for the conclusion of this CRP were discussed in RCM 3.

Given the large variety of research questions, scenarios, features, and objectives that can be potentially addressed by numerical modelling, considerable coordination was required to define topics that are suitable for collaborative research and at the same time relevant and of interest to the participating countries. Furthermore, the technical challenges related to running sophisticated simulation software and developing complex site-specific models require substantial investments in training, data analysis, and model setup, which are beyond the scope of the CRP.

The participants' responsiveness to IAEA's coordination efforts ensured that the overall objectives of this CRP have been met, even though specific aspects as outlined in the original goals were not achievable. For example, a formal calibration and validation of the developed process models was not attempted due to a lack of suitable characterization data, the inherent difficulty of developing complex, site-specific forward models, and the unavailability of suitable inverse modelling software.

In addition to numerous simulation studies and sensitivity analyses that focused on the disposal concept and hydrogeological conditions of each country, major outcomes of this CRP are the comparison studies on cross-cutting issues. They are documented in more detail in Section 4 of this report.

The following concluding remarks clarify some of the outcomes and summarize the main achievements and lessons learned from this exercise:

- A relatively large number of simulations codes were used by the participants to perform the simulation tasks of this CRP. The participants did not seem to encounter significant technical difficulties in running the simulators;
- The results of flow and radionuclide transport simulations were found to be largely independent of the particular software being used;
- Model predictions were highly sensitive to decisions about the model structure, the features implemented, and parameterization;
- The decision to go beyond a mere benchmark exercise and to conduct a challenging comparison study to examine conceptual model uncertainty proved to be ambitious. First, the design of the comparison study was difficult given the large variety of possible simulation scenarios and the correspondingly limited overlap in cases considered by the four teams. Such overlap is needed for the comparison study to yield conclusive results. The four comparison studies developed during the RCMs — while of limited scope — had the potential to provide useful insights into the reliability of model predictions; this potential was only partly realized. The second challenge faced by the comparison study was the required high level of collaboration and coordination among the participants. Small meetings in between RCMs may help facilitate interactions among the participants;
- While the flow and transport simulators used as part of this CRP did not present a technical challenge to the participants, it must be noted that only basic processes were considered. Some participants explored the use of more sophisticated simulators that can handle coupled hydrological, thermal, and mechanical processes. However, coupled biogeochemical and geophysical processes were not considered, neither was inverse modelling. Obtaining experience in advanced simulation capabilities is highly technical and best achieved through short courses and extended fellowships;
- The background, specialization, and level of expertise in numerical modelling varied considerably among the participants. This CRP benefited from the supplemental training courses in the use of specific modelling software, as well as from fellowships,

in the framework of a related TC project, which allowed some of the participants to obtain additional knowledge and experience in the use of numerical simulation tools.

1. INTRODUCTION

1.1. BACKGROUND OF THE COORDINATED RESEARCH PROJECT

The International Atomic Energy Agency (IAEA) implements research activities through Coordinated Research Projects (CRPs), which bring together research institutes in both developing and developed Member States to collaborate on research topics of common interest. The overall purpose of the CRP on "*The Use of Numerical Models in Support of Site Characterization and Performance Assessment Studies of Geologic Repositories*" was to transfer modelling expertise and numerical simulation technology to countries needing them for their national nuclear waste management programmes. This goal is achieved by:

- Efficiently disseminating modelling expertise for site characterization and performance assessment in nuclear waste isolation;
- Enabling participating Member States to implement integrated data interpretation and modelling strategy tailored to each country's repository concept and geologic conditions;
- Solving well-defined research topics of common interest to the participants.

Numerical modelling is a key component of any nuclear waste isolation programme. Simulation and optimization technologies are used to (1) improve the understanding of complex coupled processes in the subsurface, (2) integrate available characterization data into a comprehensive conceptual model, (3) design laboratory and field experiments and analyse the resulting test data, (4) reproduce the observed state of the natural system, (5) predict the performance of the proposed repository system over extended time periods, and (6) assess parametric and conceptual uncertainties in these predictions.

Basic activities as part of this CRP consisted of (1) demonstrating the use of modelling strategies to address relevant issues using site-specific data (if available), (2), gaining insights in the reliability and uncertainty of numerical model predictions, and (3) improving the modelling capabilities at institutions in the participating Member States. Resources and competence provided by the IAEA Underground Research Facilities (URF) Network [1] facilitated the transfer of knowledge and technology to developing Member States, by allowing appropriate training (and fellowships) and development of competence and assistance in some aspects of numerical modelling in the framework of an IAEA Technical Cooperation project.

IAEA awarded five Research Contracts to the following countries and institutions:

- *Brazil (BRA)*; Centro de Desenvolvimento da Tecnologia Nuclear (CDTN), Commissão National de Energia Nuclear (CNEN);
- *China (CPR)*; Beijing Research Institute of Uranium Geology (BRIUG); China National Nuclear Corporation (CNNC);
- *Lithuania (LIT)*; Lithuanian Energy Institute (LEI), Nuclear Engineering Laboratory;
- *Romania (ROM)*; Institute for Nuclear Research (SCN), Nuclear Safety and Reactor Physics Division;
- *Ukraine (UKR)*; Radio environmental Centre of the National Academy of Science of Ukraine, Department of Hydrogeological Modelling.

In addition, the following two Research Agreements were awarded:

- *India (IND)*; Bhabha Atomic Research Centre (BARC);
- *Republic of Korea (ROK)*; Korea Atomic Energy Research Institute (KAERI).

Scientific Coordinators from the following Member States supported this CRP:

- *Belgium (BEL)*; Studiecenter voor Kernenergie, Centre d'Étude de l'Énergie Nucléaire (SCK CEN) ;
- *United Kingdom (UK)*; Cardiff University, Geoenvironmental Research Centre (GRC);
- *United States of America (USA)*; Lawrence Berkeley National Laboratory (LBNL), Earth Sciences Division (ESD).

The five-year CRP started in October 2005; Phase I, which covered the period up to August 2008, was documented in various Progress Reports, Contract Reports, two Synthesis Reports, and a Mid-Term Report. These materials were consolidated in a Phase I Final Report [2] (also published externally as Ref. [3]).

1.2. OBJECTIVES

The overall purpose of this CRP was to transfer technology from Member States with advanced numerical modelling capabilities to Member States currently evaluating the use of such technologies in support of site characterization activities, design of field and laboratory experiments, data analyses by means of inverse modelling, and total system performance analyses.

The modelling approach was demonstrated and optimized by developing a numerical model suitable for predicting a specific aspect of the repository system. The issue of interest was identified by the participating Member States, and available data and information from those States were used in the demonstration. The studies focused on (1) the use of sophisticated numerical modelling tools as a means to integrate existing data into a conceptual understanding of the repository system, (2) the use of these models for predictive purposes, and (3) the development of recommendations for future test design and data collection activities, driven by the need to reduce prediction uncertainties of key components of the natural system.

The specific objectives of this CRP are for participating Member States to:

- Help the participants to develop an integrated data interpretation and modelling approach tailored to the repository concept and geologic conditions of the participating Member States;
- Acquire expertise in model-development strategies and the use of sophisticated numerical simulators for the reproduction of the observed natural system state and the prediction of the repository system behaviour;
- Become skilled at using numerical modelling tools for the design of laboratory and field experiments;
- Examine the advantages and limitations of numerical models for the study of complex coupled processes.

As a result of this CRP, the Member States will become familiar with internationally accepted simulation and analysis methods and the related computational tools, and obtain insights into the capabilities and limitations of numerical methods as used in support of site characterization and performance assessment.

1.3. SCOPE

Each Member State involved in this CRP was expected to acquire the scientific basis and to demonstrate expertise in the site characterization process including test design, data analysis, model calibration, model validation, predictive modelling, sensitivity analysis, and uncertainty propagation analysis. The acquired expertise was to be documented in a technical report in which numerical modelling is used to address a pertinent issue (selected by the Member States) using data and information from a potential repository site.

The specific activities of the CRP were for participating Member States to:

- Identify issue to be addressed by a comprehensive modelling study;
- Review existing geological, hydrological, and geochemical data and their suitability for site characterization and/or hypothesis testing;
- Analyse different types of data (hydraulic, geochemical, isotopic, thermal, seismic, etc.) for incorporation into conceptual and numerical model development;
- Perform data integration and model calibration exercises;
- Conduct, when possible, deterministic and/or stochastic model prediction including sensitivity and uncertainty propagation analyses;
- Identify key features and parameters that may need further characterization;
- Recommend test design suitable for identification of relevant features and parameters;
- Write technical reports.

Resources and competence provided by the URF Network [1] facilitated the transfer of knowledge in this field to developing Member States.

1.4. STRUCTURE

This report summarizes the research conducted by the CRP participants in the period 2005 - 2010, and discusses major findings. Section 2 describes the coordination activities of this CRP and discusses the decisions made during the Research Coordination Meetings. Section 3 contains short summaries of the objectives, activities, results, and conclusions of each participant conducting numerical simulations (more detailed descriptions of selected research activities can be found in Annexes IV-VII). The comparative analyses regarding both near field and far field modelling issues are discussed in Section 4. The main conclusions of this CRP are given in Section 5. A common, semi-generic site (modelled after the Veresnia Site in the Ukraine) was chosen as the basis for the far field simulation studies; the site is described in Annex I. Annex II contains each participating country's specifications for the waste disposal concepts and related simulation cases. Short descriptions of computer codes used in the simulations of the participants are given in Annex III. Annexes IV-VII describe complementary simulation studies based on the country-specific models that led to significant findings of general interest.

2. COORDINATED WORK PROGRAMME

2.1. MANAGEMENT OF COORDINATED RESEARCH ACTIVITIES

The IAEA URF Network [1] served as the framework for cooperative activities shared between members of the Network and participants of the CRP.

Five Research Contracts (BRA, CPR, LIT, ROM, UKR) and two Research Agreements (IND, ROK) were signed after a merit review of the proposals submitted by prospective participants of this CRP; moreover, the services of three Scientific Coordinators from BEL, UK, USA were secured (see Section 2). Research activities were coordinated by IAEA and supporting Member States at three Research Coordination Meetings (RCMs) held in Beijing, China, in September 2006, Daejon, Republic of Korea, in May 2008, and Kaunas, Lithuania, in November 2009 (see Section 2.3). Progress was evaluated at the RCMs and monitored through review of various interim reports and deliverables. Contract renewal was contingent on proposal quality and performance.

The project status was assessed in a Mid-Term Report and a Final Report for Phase I [2, 3]. In these reports, the participants' accomplishments were summarized and evaluated, decisions from the RCMs were noted, and recommendations were made regarding future interactions and research planning. Adjustments to the initial research plan were made as deemed necessary or beneficial to the overall outcome of the CRP (see 2).

2.2. EXPECTATIONS AND ADJUSTMENTS OF OBJECTIVES AND SCOPE

The general and specific objectives of this CRP (see Section 2) are challenging in that they involve the use of advanced simulation technologies to address a wide range of questions related to site characterization and performance assessment for a variety of country-specific waste disposal concepts, waste inventories, and geological formations. For this CRP to succeed, the scope of specific simulation tasks and analyses had to be flexibly defined and adjusted in accordance with attainable goals, actual accomplishments, data availability, member interests, and accessible resources at the participating institutions. This coordination was mainly achieved during the three RCMs (see Section 2.3) and through recommendations made in status reports [2, 3]. Moreover, interim project reports were exchanged among the participants.

The interests expressed in the initial proposal by each selected participating Member State reflected the respective repository system and host formation, specific issues of concern, and available software. The submitted CRP proposals can be categorized as follows:

1. *Capability development* (specifically, studies supporting code selection and development of specific modelling capabilities): CPR, ROM, ROK, IND;
2. *Code application* (specifically, radionuclide transport studies for site selection): UKR, LIT;
3. *Theoretical studies* (specifically, related to total system performance assessment (TSPA)): BRA, CPR, ROK.

Based on these differences and common interests, test cases and comparative studies were identified during the first RCM (see Section 2.3.1) to arrive at a coordinated and collaborative research programme.

Work performed during the first year of the CRP was documented by each participant in short progress reports (delivered August 2006), providing insights into the repository systems and simulation approaches considered by each participant. The progress reports were reviewed by IAEA and the CSIs, resulting in observations, questions, and suggestions that were discussed with the participants. While progress had been made towards the project objectives, a clear strategy for site characterization, data analysis, model development, sensitivity and uncertainty analyses was missing in most cases. This issue was addressed in the first RCM, resulting in a coordinated effort to focus on a set of common objectives, and by developing common cases to be jointly examined by all participants. In particular, two groups were formed: Group A focused on process modelling issues, whereas Group B examined alternative TSPA methodologies, one based on probabilistic and the other a possibilistic (fuzzy logic-based) approach.

A second progress report, submitted in August 2007, described the work conducted during the second year of the CRP. Overall, the participants responded to the project redirection implemented during the first RCM. Progress was made on most assignments, with additional activities identified and recommendations made in the Mid-Term Report. The research plan for Year 3 was developed. It included short term tasks that were proposed to ensure that the objectives of Phase I (Years 1–3) of this CRP were met.

The second RCM (see Section 2.3.2) further evaluated the accomplishments and identified gaps that needed to be filled in order to complete a meaningful comparative analysis. Detailed recommendations and assignments were made, with results expected to be included in five country-specific contract reports and two group-specific synthesis reports (submitted August 2008), which document the work conducted during Phase I of the CRP, summarized in Refs [2, 3].

Recommendations made at the end of Phase I provided the basis for the planning of Phase II (Years 4 and 5). It was found that not sufficient information was present (or likely to become available in a timely manner) to continue the investigation of the possibilistic TSPA approach analysed by BRA. Consequently, the contract with BRA was not renewed for Phase II, requiring an adjustment of the comparative work conducted in Group B and its interaction with Group A. This readjustment and the definition of work for the conclusion of this CRP was discussed in RCM 3 (see Section 2.3.3).

Given the large variety of research questions, scenarios, features, and objectives that can be potentially addressed by numerical modelling, considerable coordination was required to define topics that are suitable for collaborative research and at the same time relevant and of interest to the participating countries. Furthermore, the technical challenges related to running sophisticated simulation software and developing complex site-specific models require substantial investments in training, data analysis, and model setup, which are beyond the scope of the CRP (but partly supported by other IAEA programmes).

The participants' responsiveness to IAEA's coordination efforts ensured that the overall objectives of this CRP have been met, even though specific aspects as outlined in the original goals were not achievable. For example, a formal calibration and validation of the developed process models was not attempted due to a lack of suitable characterization data, the inherent difficulty of developing complex, site-specific forward models, and the unavailability of suitable inverse modelling software.

In addition to numerous simulation studies and sensitivity analyses that focused on the disposal concept and hydrogeological conditions of each country, major outcomes of this CRP were the comparison studies on cross-cutting issues. They are documented in more detail in Section 4 of this report.

2.3. RESEARCH COORDINATION MEETINGS

This CRP aimed at leveraging on the expertise and modelling capabilities of each participating country. Exchange of technical information as well as comparative analyses were integral parts of this approach. Coordination of activities and the development of joint work scope were thus essential and the main objectives of the RCMs. The following subsections summarize the results of the three RCMs held as part of this CRP. The decisions made at these RCMs were reflected in the scope proposed in the annual contract renewals.

2.3.1. RCM 1, Beijing, 2006

The first Research Coordination Meeting was held in Beijing, China, from 11 to 15 September 2006. The main purpose of the meeting was for the participants to report on first-year accomplishments, to discuss the proposed research plans, and to coordinate the activities. The presentations given by each CRP participant highlighted the diversity of repository concepts and host formations considered for disposal of nuclear waste, as well as the variety of characterization approaches and simulation tools used to predict long-term performance. The discussions also revealed common interests (e.g. in code selection, predictive modelling, and TSPA strategy) and challenges (e.g. prediction of coupled processes on multiple scales, availability and inclusion of characterization data, and the quantification of uncertainties).

In an effort to coordinate the research, to foster collaboration among the participants, and to better align the project with the overall goals of the CRP, two main topics of common interest were identified — process modelling and total system performance assessment (TSPA) methodology, and two groups were formed as follows:

2.3.1.1. Group A: Process modelling

Main objectives:

(1) Develop and use numerical process model of semi-generic site to support site characterization and performance assessment;
(2) Perform sensitivity analyses to identify key parameters, features, and processes;
(3) Examine uncertainty resulting from differences in conceptual model, scenario, and supporting data;
(4) Provide simulation results to Group B.

Group members:

CPR (lead), LIT, ROM, UKR; support from IND, ROK

General approach:

(1) Develop a process model of a semi-generic site based on a description of the Veresnia site provided by UKR; additional generic data and their uncertainties were provided by CPR based on borehole data from Beishan;
(2) Near Field: Describe generic repository system based on the Swedish concept (LIT); identify key radionuclides and source term (ROM);

(3) Far Field: Develop three alternative conceptual models of the geosphere; Model 1: Porous medium model (LIT, UKR); Model 2: Porous medium model with discrete features (ROM); Model 3: Discrete fracture network model (ROK);
(4) Perform process model simulations of groundwater flow and radionuclide transport; calculate performance measures at potential compliance boundary; conduct sensitivity analyses;
(5) Compare simulation results to assess prediction uncertainties;
(6) Provide simulation results (source term, radionuclide release rate from engineered barrier system (EBS), radionuclide flux at compliance boundary) to Group B.

2.3.1.2. Group B: TSPA methodology

Main objectives:

(1) Demonstrate total system performance assessment (TSPA) methodology by developing simplified TSPA model;
(2) Compare alternative TSPA methodologies:
   — Methodology 1: Probabilistic assessment using Monte Carlo simulations (CPR);
   — Methodology 2: Possibilistic assessment using fuzzy logic (BRA);
(3) Provide results of impact analysis to Group A.

Group members:

BRA (lead), CPR

General approach:

(1) Define components of repository system to be included in simplified TSPA model;
(2) Develop simplified TSPA model for radionuclide migration analysis;
(3) Select key parameters and their uncertainty distributions;
(4) Define performance measure;
(5) Run TSPA model and compare results;
(6) Identify key parameters as well as key features, events, and processes (FEPs) affecting repository performance and report to Group A.

2.3.2. RCM 2, Daejon, 2008

The second Research Coordination Meeting was held in Daejon, Republic of Korea, from 19 to 23 May 2008. The main purpose of the meeting was for the participants to report on the accomplishments since the last RCM, specifically addressing the technical and coordination issues raised and recommendations made in the Mid-Term Report (see Ref. [2]). The presentations given by each CRP participant, the ensuing discussions, and the decisions can be summarized as follows:

(1) The participants largely adhered to the recommendations made in the Mid-Term Report, as provided in Ref. [2];
(2) The organization of the CRP in two groups (Group A: Process modelling, and Group B: TSPA methodology) helped focus and integrate the projects, and fostered collaboration;
(3) The cases and scenarios of interest to individual countries differ from the illustrative case to be examined as part of the CRP;

(4) To enable successful completion of Phase I of the CRP, technical information was exchanged, scenarios defined, and a schedule with milestones and deliverables defined; specifically:
   (a) Data and simulation results needed for the illustrative case and the subsequent comparison study (in which differences in model predictions and TSPA results were evaluated in the light of differing input assumptions and alternative computational methods) were to be prepared and exchanged;
   (b) Each participant wrote a final report (Contract Report) in its individual CRP project;
   (c) Each group wrote a Synthesis Report that summarized the illustrative case results and the comparison study.

The following decisions were made concerning the remainder of Phase I of the CRP.

2.3.2.1. Group A: Process modelling

- Develop illustrative case as basis for comparison study;
- Perform comparison study to assess impact of assumptions on source term scenario, model conceptualization, and parameter values on repository performance;
- Illustrate coupled process models for near field and far field using country-specific data and simulations.

2.3.2.2. Group B: TSPA methodology

- Use a simplified system description for the TSPA analysis;
- Use TSPA far field input parameters consistent with Group A's illustrative case;
- Calculate specific performance measures suitable for a comparison study;
- Perform probabilistic and possibilistic TSPA simulations.

Based on these decisions, country-specific Contract Reports as well as two Synthesis Reports were developed, as summarized in Ref. [2].

2.3.3. RCM 3, Kaunas, 2009

The third Research Coordination Meeting was held in Kaunas, Lithuania, from 9 to 13 November 2009. The meeting included technical presentations by the Research Contract holders (CPR, LIT, ROM, and UKR), the Research Agreement holder (ROK), and the scientific coordinators, followed by discussions of research results and planning of activities for the final year of the project. Visits of Lithuanian Energy Institute (LEI) laboratories and the Maišiagala nuclear waste storage facility were organized. Social events were sponsored by LEI and IAEA.

The purpose of the meeting was to review the progress of activities within the CRP and to coordinate short term actions in accordance with the Phase II goals. The work to be performed for the final year was restructured in response to the discontinuation of the contract with BRA, which rendered a comparative analysis of probabilistic and possibilistic performance assessment analyses unfeasible.

Based on a summary list of simulation cases, objectives were identified suitable for a comparative analysis. Four comparison studies were developed: Two studies relate to near field behaviour aimed at examining (a) how the conceptual model and the choice of computer code affected release curve calculations, and (b) how differences in the disposal concept lead to different radionuclide releases from the engineered barrier system; and two comparative studies of far field simulations examined (c) the impact of the geosphere conceptualization on predicted radionuclide break through curves, and (d) the differences between detailed process simulations and abstracted TSPA model predictions.

Performance measures suitable for the comparison studies were defined, lead authors for each study identified, and a schedule and deliverables worked out so that the comparison studies could be included as a main component of the Final Report of this CRP.

3. SHORT SUMMARIES OF RESEARCH ACTIVITIES

Each participant conducted a variety of numerical simulation studies to address country-specific issues and to contribute to the general objectives of the CRP, which required model runs in support of the comparative analyses to be discussed in Section 4. The following subsections highlight the main objectives, activities, results, and conclusions of the research conducted by each participating Research Contract holder (CPR, LIT, ROM, and UKR); more details can be found in Annexes IV-VII as well as the previous project and status reports. The specifications for these four countries can be found in Annex II.

The Research Agreement holders (IND and ROK) contributed to the scientific investigations in an informal way. Some simulation results from ROK are included in the discussions of the comparison studies (see Section 4). IND contributed to the RCMs mainly by sharing expertise in the simulation of coupled thermo-hydrologic-mechanical processes. Coupled-process simulations were not considered in the comparison studies; therefore, IND's contributions are not reflected in this report.

3.1. CHINA

The main objectives of the CPR project were (1) to understand the total system performance assessment (TSPA) process, (2) to gain understanding of the advantages and limitations of numerical modelling, and (3) to improve the skills of using the GoldSim[1] [4] system-level modelling tool. Moreover, CPR led the comparison study on the impact of far field modelling approach (Section 4.4.1), and contributed to the comparison study on the impact of the conceptualization of the geosphere (Section 4.3).

In the first two years, CPR focussed on learning the theory of different TSPA approaches and the use of the GoldSim code. Next, process model simulations were performed, and the TSPA approach was applied using a generic geological disposal model. Sensitivity and uncertainty analyses were conducted, which identified flow velocity, fracture length and aperture, and the matrix diffusion coefficient as the most sensitive parameters with respect to the radionuclide concentration in the river as well as the dose rate.

In the following two years, CPR cooperated with other countries within the CRP framework to carry out the comparison study. Specifically, deterministic and probabilistic simulations of the reference case were performed to study the impact of the simplifications needed for a TSPA analysis on model predictions.

While it is recognized that the TSPA framework and GoldSim model developed as part of this CRP is very preliminary, the expertise gained is considered useful for the future development of a TSPA model for the assessment of China's geological disposal system.

Its results can be used to help design future tests and data collection activities, and to reduce prediction uncertainties of key components of the natural system. As an important outcome of this CRP project, CPR established a group specialized in numerical modelling

[1] The computer codes used in this CRP have been referenced where they first appear in the main text and listed alphabetically, also with references, in Annex III.

3.2. LITHUANIA

The main objectives of the LIT project are (1) to assess radionuclide transport in the near field, (2) to analyse groundwater flow and radionuclide transport in the far field, and (3) to perform numerical modelling of the coupled processes in the near field. Moreover, LIT led the comparison study on the impact of the near field model conceptualization (Section 4.1.1) and contributed to the comparison study on the impact of the disposal concept (Section 4.2.1) and on the impact of the conceptualization of the geosphere (Section 4.3).

The modelling of near field releases was performed for a generic repository concept based on the disposal of RBMK-1500 spent nuclear fuel in crystalline rocks. The analysis of the near field releases included various canister-defect and climate-change scenarios. For the modelling of the groundwater flow and the radionuclide transport, a porous medium approach and the conceptual model of the semi-generic Veresnia site were used. Different groundwater flow regimes were investigated, and their impacts on the ^{129}I release at the discharge points (well, river) have been estimated.

Coupled process models were used to investigate (1) the influence of heat and gas generation on radionuclide transport, and (2) the impact of coupled thermal-hydrological-mechanical processes on the behaviour of engineered barriers.

The results of the near field modelling releases using base-case parameters were compared to those of other modellers in order to evaluate the sensitivity of conceptual model, the choice of the computer code, and the disposal concept.

As expected, simulations using similar conceptual models yielded consistent results, irrespective of the computer code used. However, the results are sensitive to changes in the conceptual model and the way the coupled processes are included.

3.3. ROMANIA

The main objectives of the ROM project are (1) to determine the source term using a variety of codes and conceptual models, (2) to simulate groundwater flow and radionuclide transport in the far field, and (3) to study the influence of coupled thermal-hydrologic effects on the temperature distribution in the repository. Moreover, ROM led the comparison study on the impact on the impact of the disposal concept (Section 4.2.1), and contributed to the comparison study on the impact of the conceptualization of the geosphere (Section 4.3) and on the impact of far field modelling approach (Section 4.4.1).

ROM based its repository model on the Canadian concept, which was represented as a 1D source term using the codes GRAPOS1 (a module of German assessment code EMOS [5]) and DUST-MS [6]. Two types of far field simulations were performed: A 2D FEFLOW [7] model of flow and transport through porous and fractured media, and a 1D model using the code CHETMAD (a module of EMOS [5]). The influence of the source-term boundary conditions on contaminant fate was investigated using 1D simulations of the near field with the DUST-MS, and 2D flow and transport calculations with PORFLOW [8].

Both the near and far field studies demonstrated the significance of the boundary conditions on predicted radionuclide breakthrough curves. Considering the coupled thermal-hydrologic effects impacts the maximum temperature in the repository, which in turn may affect the performance of the engineered barriers.

3.4. UKRAINE

The main objectives of the UKR project are (1) to perform radionuclide transport simulations in support of a site suitability analysis for a geological repository within the Chernobyl exclusion zone and adjacent territories, (2) to determine additional data needs, and (3) to learn from international experience in applying numerical simulations in support of site characterization and safety assessment of geological disposal of nuclear wastes. Moreover, UKR provided the description of the semi-generic site used for the comparison studies (Annex I), led the comparison study on the impact of the conceptualization of the geosphere (Section 4.3), and contributed to the comparison study on the impact of far field modelling approach (Section 4.4.1).

A conceptual model and a corresponding numerical 2D regional flow and transport model were developed, representative of the Ukrainian generic site. An equivalent porous medium model including a discrete fracture zone was used. Flow and transport simulations were performed using the PMPath code [9]. The base-case scenario considers radionuclide release from a single defect canister, starting immediately after waste emplacement. The flow fields and corresponding advective transport times from the repository to two discharge points (river and well) were determined along with relative contaminant concentrations for varying well drawdowns, boundary heads, sorption coefficients, and hydraulic conductivities. Moreover, the impact of the fracture zone (and its conductivity) was analysed. Flow rates, relative concentration fluxes, and cumulative release curves for ^{129}I at specified control points within the model domain were calculated.

It was concluded that the boundary conditions (prescribed fixed heads at the river and well locations) have a dominant impact on the flow field within this confined model domain, and thus greatly affect radionuclide migration, breakthrough times, and relative concentrations. Furthermore, changes in hydraulic conductivity affect the shallow and deep convection pattern, leading to significant changes in predicted transport behaviour. Changes in fracture hydraulic conductivity and sorption coefficient have the expected effect on radionuclide concentrations in the river or well. The calculated travel times significantly depend on geosphere hydrogeological input parameters. Furthermore, the radionuclide fluxes as well as peak and cumulative concentrations depend on the chosen release scenario, resulting in many orders-of-magnitude differences in the predicted dose.

The simulations suggest that the repository should be placed in locations where vertical downward movement of groundwater dominates, and where a sedimentary cover and granite weathering crust are present. The results of the project may be used later for establishing site selection criteria and for developing national capabilities in safety assessment.

4. COMPARISON STUDIES

The overall purpose of the comparison studies described in this section is to evaluate the impact of specific aspects of (1) the repository system itself or (2) its representation in a numerical model on predicted performance measures such as radionuclide concentrations at a compliance boundary. Unlike a standard parametric sensitivity analysis, evaluating these aspects requires a comparison of different conceptual models. The CRP framework provides an opportunity to examine different disposal concepts and different modelling approaches as part of a Coordinated Research Project that defined common performance measures. Four comparison studies were conducted as part of this CRP, two related to the simulation of the near field and calculation for radionuclide releases from the engineered barrier system, and two related to radionuclide transport from the repository through the geologic far field to a compliance boundary. The four analyses, each led by a separate participant, are summarized in the following subsections.

A common performance measure was defined as the object of model comparison. Normalized cumulative releases from the repository and to the compliance boundary are being examined for ^{79}Se and ^{129}I, two radionuclides that are considered representative for a number of performance-relevant contaminants regarding their half-life, sorption behaviour, and solubility. ^{129}I is long lived, very soluble and weakly sorbing. ^{79}Se is much more influenced by radioactive decay for the simulation time of 10^6 years, strongly sorbing, and almost insoluble. Normalization removes the differences in the assumed inventory.

4.1. IMPACT OF NEAR FIELD CONCEPTUAL MODEL AND CODE

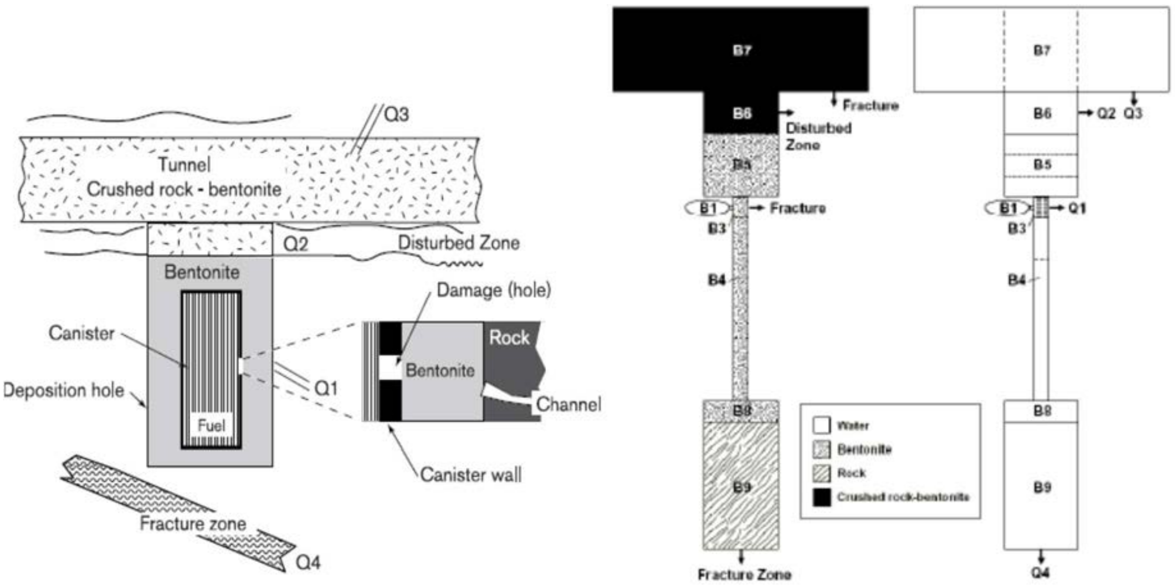
4.1.1. Objectives

The objective of this comparison study is to evaluate the sensitivity of the conceptual model and computer code on the near field release of ^{79}Se and ^{129}I. Normalized cumulative release curves for these two radionuclides at the bentonite/host rock interface were calculated. This comparison study was performed by LIT with input from CPR, LIT and ROK.

4.1.2. Case description

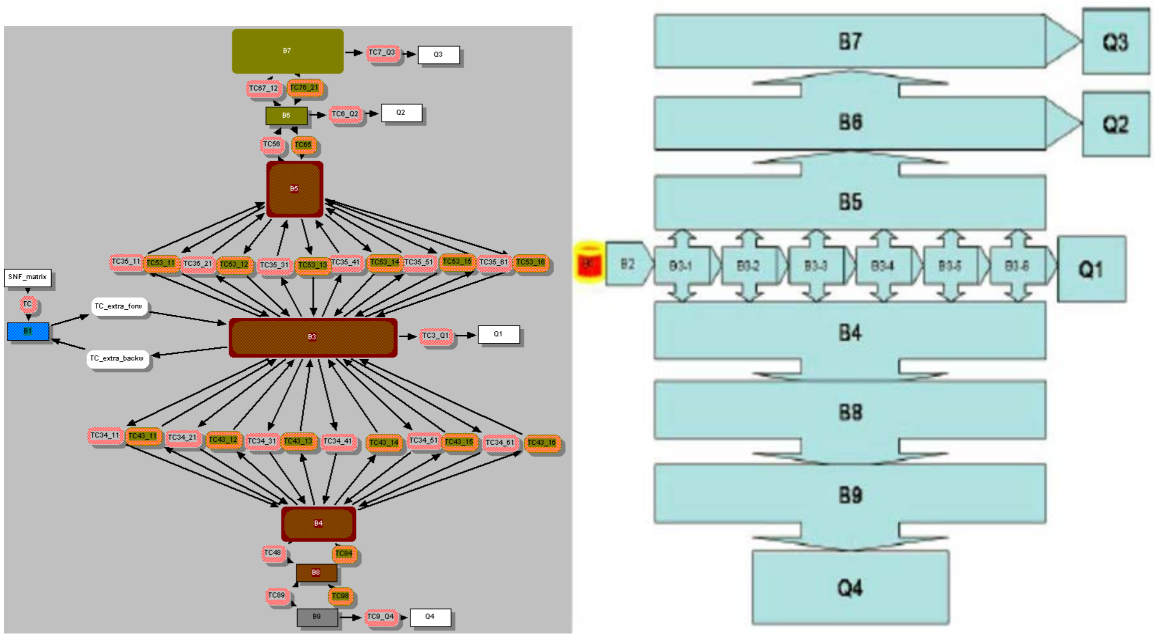
The modelling of radionuclide migration in the near field was examined for a repository that is based on the Swedish KBS-3V concept. A schematic view of the near field, possible radionuclide release paths to the host rock and the corresponding conceptual model are shown in Fig. 1.

LIT used the AMBER code [10], whereas CPR and ROK used GoldSim [4] for the modelling of radionuclide release from the near field. Both of these codes use a compartment approach, in which mass is transferred between the compartments, and contaminant sinks/sources are provided for each contaminants. The implementations of the simplified conceptual near field models in AMBER and GoldSim are shown in Fig. 2. The base case parameter set used for comparison study calculations is discussed in Ref. [11].



(a) (b)

FIG. 1. Schematic view of (a) the near field, including various transport paths from the repository to the host rock and (b) the corresponding conceptual model.



(a) (b)

FIG. 2. Simplified near field models as implemented in (a) AMBER by LIT [11], and in (b) GoldSim by CPR [12].

4.1.3. Simulation results

All three teams performed simulations for different types of SNF, i.e. for the inventory typical to the respective country (see Annex II). Only two radionuclides, ^{79}Se and ^{129}I, are considered for the comparison study. In order to have results in comparable form, the cumulative release rates are normalized by the initial amount of radionuclides in spent nuclear fuel to account for the different inventories of ^{79}Se and ^{129}I in RBMK-1500, BWR and CANDU SNF. The results obtained by LIT, CPR and ROK are presented in Fig. 3.

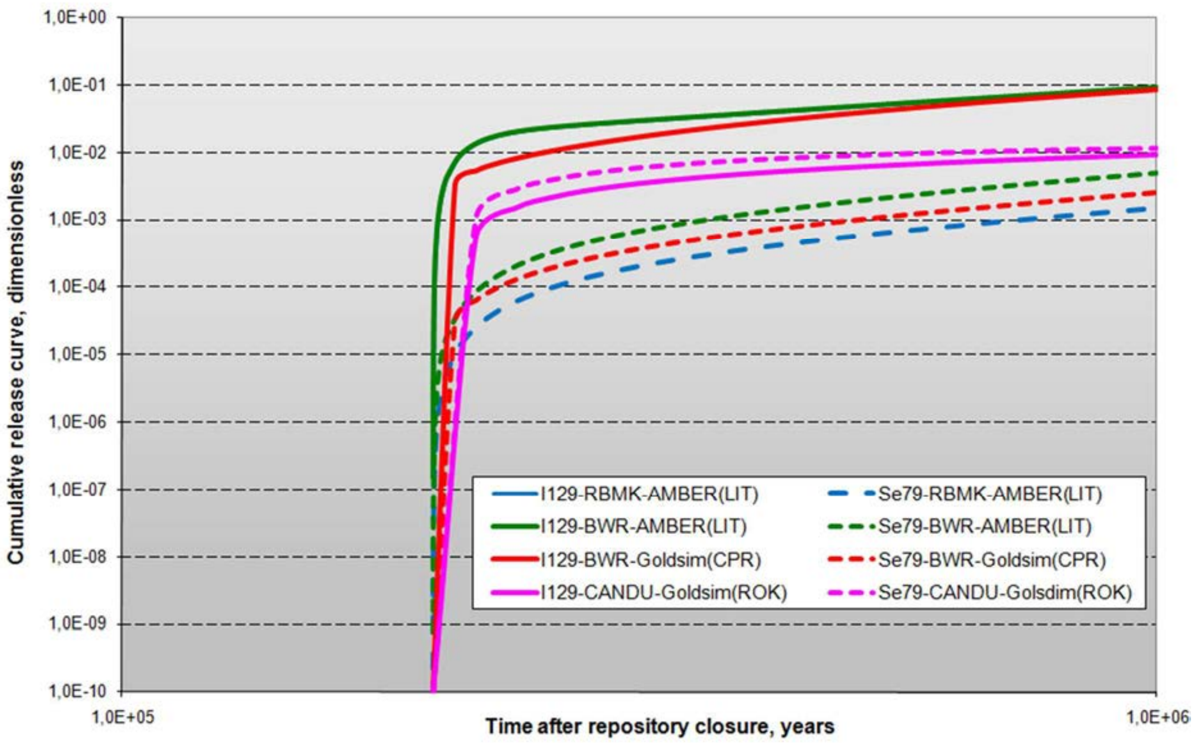


FIG. 3. Cumulative release (normalized to initial inventory) from the near field.

4.1.4. Comparative analysis

The simulation results contributing to this comparison study are affected by the fact that different SNF inventories were used. This leads to different amounts of radionuclides being released from the canister, because the instant release fraction and the amount of radionuclide release from the SNF matrix are both a function of the inventory. As radionuclides are released from the canister mainly by diffusion, the release rate depends on the concentration gradient between the canister and the surrounding bentonite. On the other hand, the amount of radionuclides released from SNF is not a determining factor if the release from the canister is governed by the solubility limit.

As shown in Fig. 3, the normalized cumulative release curves for ^{129}I — obtained using the same methodology and computer code (AMBER) — are very similar, irrespective of whether the radionuclide is released from BWR or RBMK SNF. Thus, for the radionuclide whose release is not determined by the solubility limit, normalization eliminates the difference in the initial inventory. However, this is not the case for ^{79}Se, whose cumulative release curves are different for RBMK and BWR SNF despite normalization. The cumulative release curve of ^{79}Se released for RBMK SNF is lower than that for BWR SNF by a factor of approximately 3.4. If ^{79}Se release is determined by solubility limits, the release rate curves are the same for BWR and RBMK SNF, but normalization to different initial inventories leads to the noted difference.

Fig. 3 shows that the results obtained by LIT and CPR correlate quit well, while the results obtained by ROK differ more significantly. The small differences between the results of LIT and CPR are attributed to the different mathematical models for radionuclide release and transport implemented in AMBER and GoldSim. In general, however, the consistency of the conceptual model (instant release from SNF and subsequent release though the bentonite barrier) together with low sensitivity of the results to the numerical scheme implemented in the computer code, and low sensitivity to initial inventory leads to overall consistency in the simulation results.

The release of ^{129}I predicted by ROK is about one order of magnitude lower than that observed by LIT and CPR, while the release of ^{79}Se is approximately one order of magnitude higher than that calculated by LIT and CPR. Also the release of ^{79}Se obtained by ROK is larger than that of ^{129}I for the considered time period.

4.1.5. Conclusions

The consistency between the results obtained by LIT and CPR indicate similarity in the conceptual model and low sensitivity to the computer code and its numerical scheme. The results obtained by ROK (even though calculated with the same code as that used by CPR) are fundamentally different in the predicted relative release of ^{79}I and ^{129}I, even though their absolute values are within one order of magnitude of those obtain by the other participants of the comparison study.

This outcome highlights that model conceptualization tends to have a much larger impact on simulation results than differences in computer codes and their respective solution methods.

4.2. IMPACT OF DISPOSAL CONCEPT ON NEAR FIELD BEHAVIOUR

4.2.1. Objectives

The objective of this comparative study is to assess the impact of the disposal concepts on releases from the repository. This comparison study was performed by ROM with contributions from CPR, LIT, ROK and ROM.

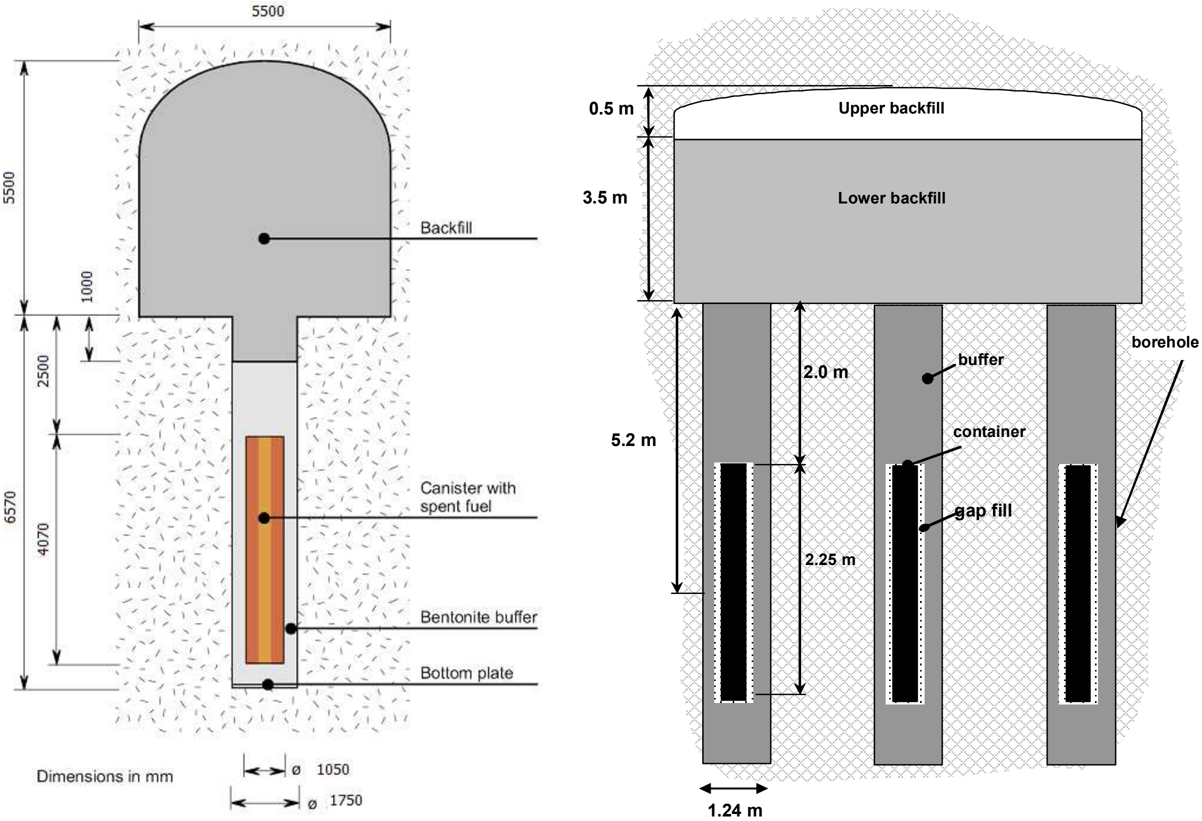
4.2.2. Case description

There are large differences in the various concepts considered for the disposal of spent nuclear fuel, from the fuel type and inventories, to container design, to repository layout; these differences affect the chosen modelling approach. A summary of the modelling methodologies and most relevant data is given here to highlight the differences that might influence the interpretation of the results.

LIT studied the radionuclides used in the safety assessment of the Swedish repository. The inventory was estimated after 50 years cooling time for RBMK-1500 type fuel with a burnup of 29 MWd/kgU. ROM made a conservative estimate of the inventory from four CANDU 6 reactors, with a burnup of 7.928 MWd/kgU, considering 40 years of operation for each reactor. The total number of SNF bundles was 812 160, corresponding to 15 397 t of uranium. CPR and ROK used the fuel types PWR and CANDU respectively, and inventories provided by LIT and ROM.

The LIT repository concept for SNF disposal is based on the repository concept developed in Sweden for SNF disposal in crystalline rocks (KBS-3). The SNF disposal canister is composed of an outer corrosion copper vessel and a cast iron insert with channels for the fuel half-assemblies. Thirty-two half-assemblies (fuel bundles) of RBMK-1500 SNF could be accommodated in one disposal canister. Preliminary assessment shows that the reference canister would be 1050 mm in diameter and 4070 mm in length. In total, 1400 canisters would be required for the disposal of Lithuanian SNF. ROM considered 11 280 titanium containers, which are 2.246 m long and have a diameter of 0.63 m. One container has 72 fuel-bundles of CANDU spent fuel. CPR and ROK used KBS-3 disposal containers. The canisters are deposited either in vertical boreholes drilled into the floor of a system of deposition tunnels, or in horizontal boreholes drilled into the walls of the disposal rooms. Each hole contains one canister. The canisters are surrounded by a 37 cm thick bentonite clay buffer. Fig. 4(a) shows a cross-section through a vertical canister deposition.

ROM used the Canadian disposal concept, in which containers are emplaced in boreholes vertically drilled into the floors of the rooms, surrounded by a 25 cm thick bentonite buffer with gap-fill materials in the void spaces between the container and the bentonite. The disposal rooms are filled with two different types of bentonite, placed in layers. The disposal concept is depicted in Fig. 4(b.)



(a) LIT concept *(b) ROM concept*

FIG. 4. Cross-section of deposition holes.

One-dimensional source-term calculations were performed by LIT and ROM, using the codes AMBER and GRAPOS1, respectively.

LIT invoked the following assumptions in modelling the release of radionuclides from the repository (see also Fig. 1(a)):

(1) One defective container out of 1400 intact containers; small initial defect that grows with time. After 200 000 years, the defect is large enough to allow water to freely enter the containers;
(2) After the defect becomes larger, the entire void volume in the canister (approximately 0.5 m^3) is filled with water. Radionuclides released by SNF dissolution (by instant release of the fuel gap fraction and concurrent dissolution of the matrix and metallic parts) are dissolved in the water existing in the canister. The dissolved radionuclide concentrations are homogeneously distributed in the void volume, and are subjected to solubility limits. Sorption on the internal parts of the canister is neglected;
(3) The dissolved radionuclides slowly diffuse out through the pinhole into the bentonite buffer. The buffer is fully saturated at the time when the release of radionuclides starts. Radionuclides are transported through the bentonite buffer mainly by diffusion. Sorption onto the buffer and radioactive decay decrease the amount of contaminants in solution;
(4) Radionuclides that reach the boundary of the bentonite buffer diffuse into the water flowing in the fracture that intersects the emplacement tunnel.

ROM used the following assumptions in modelling of the source-term releases:

(1) All containers fail simultaneously after 500 years. The void volume inside the container (approximately 0.319 m^3) is instantly filled with water, and the dissolution of the matrix and metallic parts of the fuel starts. For the gap inventory, an instantaneous release is assumed, whereas the metallic part and the fuel matrix dissolves at a constant degradation rate. The homogeneously distributed dissolved radionuclide concentrations are controlled by the elemental solubility limits;
(2) The dissolved radionuclides diffuse into the 25 cm thick bentonite buffer without consideration of solubility limits. Sorption is considered. Diffusion is considered to be 1D radial;
(3) An excavation disturbed zone (EDZ) of defined cross-sectional area around the bentonite buffer is assumed, where advective flow with the groundwater takes place. At the interface between the bentonite and the EDZ, which is intersected by water-conducting features of the granitic rock, the "mixing tank" boundary condition is used, where the diffusive flux across the bentonite-host rock interface is equal to the mass flux by advection in the EDZ;
(4) The source term is strongly dependent on the water balance in the repository, and the flow rate through the entire repository is evaluated using the far field model. The groundwater flow through the repository is divided into a contaminated and a non-contaminated part. The volumetric flow through the EDZ of a container is calculated by dividing the contaminated flow fraction by the number of containers. It is assumed that the flow direction is perpendicular to the level of the repository. Contaminant transport through the EDZ takes place by advection only.

Comparison of the results assumes that the two modelling approaches properly represent the similarities in the repository concept (namely, disposal in boreholes surrounded by bentonite, one-dimensional diffusive contaminant transport through the bentonite rings, contaminants passing into the flow domain through fractures intersecting the disposal field). However, there are also substantial differences in the geometrical features, inventory and modelling strategies. Thus, in the LIT model, the container degradation is a slow process that occurs around 200 000 years after emplacement. Only one container is defective. By contrast, in the ROM model, all containers fail at once, 500 years after emplacement. Instant release fractions are also different: 8% for ^{129}I and ^{79}Se for the ROM source term, compared to 3% for ^{129}I used by LIT. The matrix dissolution rates are also significantly different. RBMK-1500 fuel has a very low dissolution time (10^7 years), whereas CANDU fuel is assumed to be dissolved in 10^4 years. The bentonite buffer is around 10 cm thicker in the LIT model. Finally, the release from the near field is influenced by the flow field at the repository level in the ROM concept.

4.2.3. Simulation results

The normalized cumulative releases of ^{129}I and ^{79}Se from the repository for the reference scenarios are shown in Fig. 5.

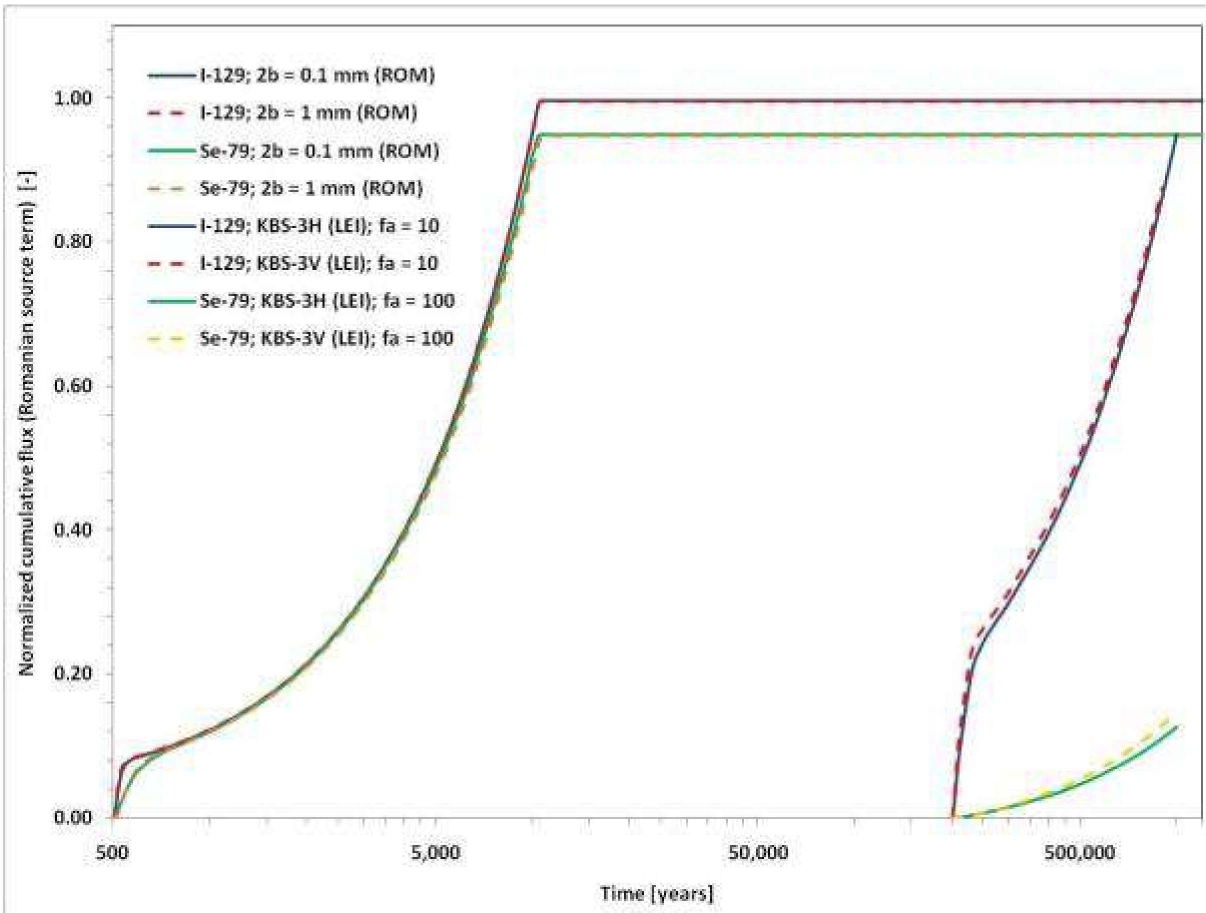


FIG. 5. Normalized cumulative release of ^{129}I and ^{79}Se from the near field; for the LIT (LEI) source-term (vertical (KBS-3V) and horizontal (KBS-3H) emplacement), the normalized cumulative release rates of ^{129}I have been adjusted by a factor f_a = 10, while the corresponding results for ^{79}Se are adjusted by a factor of f_a = 100.

The ROM source term takes into account the effect of the groundwater flow through the excavation disturbed zone (EDZ). Radionuclides diffusing through the buffer zone are carried away by the water flowing into the EDZ. The water flux into the EDZ is assumed to be one tenth of the water flowing through the active part of the repository (i.e. the disposal boreholes). The values of the groundwater flow through the EDZ, Q_{EDZ} , of the repository and through the fractures were deduced from the values of the specific discharge at the bottom of the repository, calculated with the FEFLOW code. The specific discharge at the bottom of the repository varies from 27.56 m/y in the thin fracture, and 45.99 m/y in the large fracture that intersects the disposal boreholes. Thus, an increase of 10% in the fracture aperture yields a 17% higher flow rate (from 2.76×10^{-3} m^3/y to 4.6×10^{-2} m^3/y). The release rates are affected too. The increase of the flow rates determines an increase in the release rates for both nuclides (24% for ^{129}I, and 31% for ^{79}Se), which are also narrowed at early times (up to 600 years for ^{129}I, and 900 years for ^{79}Se). After these times, the release rates show no sensitivity to the flow rate. At the end of the scenario, at 10^6 years, 99.6% of the ^{129}I and 94.9% of ^{79}Se are released from the repository for the thin fracture case, while for the large fracture the release is slightly different: 99.7% of ^{129}I and 94.8% of ^{79}Se. The releases of both nuclides show a very small sensitivity to flow rate: an increase of 17% in the flow rate leads to an increase in the normalized released mass of the non-sorbing and long lived ^{129}I with 0.1% and a decrease of 0.1% for sorbing nuclides, with lower half-lives. The influence of the flow rate is visible only at early times (up to 1% of the normalized released mass), between 100 to 300 years after container failure, when the instantaneous peak release reaches the outer boundary of the buffer. During this time, due to sorption, ^{79}Se is accumulating in the buffer, and the concentration gradient at the buffer boundary is decreasing. The buffer-rock interface is governed by a mixing tank boundary condition, which imposes that the diffusive flux at the buffer-rock interface to be balanced by the advective flow in the EDZ. Initially, the concentration gradient between the buffer boundaries is very high, which determines high influxes into the buffer. With continuous inflow, the radionuclides accumulate into the buffer, and the concentration gradient is consequently reduced. The accumulation is more pronounced for sorbing radionuclides. When the EDZ water flux is increased, the process is faster at early times, but also the mass accumulation takes place faster, so in the end the concentration gradient drops earlier. Thus, the mass release is diminished, and the effect is more important for sorbing radionuclides.

The released mass is less than the initial inventory in the container for ^{79}Se, due to its lower half-life.

4.2.4. Comparative analysis

The results plotted in Fig. 5 show that the modelling assumptions greatly impact the predicted release from the repository. The released quantities show differences of two orders in magnitude for ^{129}I, and three orders in magnitude for ^{79}Se.

For the ROM model, the release of the inventory of ^{129}I occurs much earlier compared to the release calculated by the LIT model. The entire initial quantity of ^{129}I is removed from the repository after about 10 000 years, when the waste matrix is completely dissolved. The bentonite buffer provides a weak barrier for this non-sorbing nuclide. The differences in the water flux in the EDZ play an insignificant role, and only for a short period given the variations considered in the analysis. In the LIT model, the release starts much later, around 200 000 years. At the end of the simulation, at 1 000 000 years, only 9% of the initial inventory leaves the repository. The emplacement option (vertical vs. horizontal) has no influence on the released quantity.

Based on the ROM source term model, 95% of the initial inventory of ^{79}Se leaves the repository after 10 000 years. The rest decays or is sorbed in the buffer. The flow regime in the EDZ plays a minor role in this release rate. In the LIT model, after the start of the release at 200 000 years, the quantity of released ^{79}Se increases progressively up to 0.14% for the vertical emplacement option, and 0.12% for the horizontal emplacement scenario at the end of the simulation period.

At the beginning of the release process, the increase of the released mass of ^{129}I is abrupt in both approaches as a result of specifying an instantaneous release fraction. The release is faster in the ROM model, explained by the differences in the matrix dissolution rates, which are three orders of magnitude higher. In the case of ^{79}Se, the fast increase at the beginning of the release is also due to the instant release from the fuel gap, an effect not observed in the LIT model.

4.2.5. Conclusions

The assumption regarding the time of the container failure explains the differences in the start of the release from the repository.

The waste dissolution rates play an important role in the removal of the contaminants from the repository. The emplacement option (vertical vs. horizontal) only leads to a small difference in the amount of radionuclides released from the repository.

In the current model, the flow regime within the EDZ has a minor impact on contaminant release. The influence is restricted to a few hundred years after the start of release.

4.3. IMPACT OF GEOSPHERE CONCEPTUALIZATION

4.3.1. Objectives

This comparison study was led by UKR, with contributions from LIT, ROM, CPR, and ROK.

The evaluation of geosphere conceptualization is aimed at obtaining a more complete conceptual understanding of the geological medium as a complex natural barrier system which provides, along with local (near field) engineered barriers, the safety of a deep geological repository in a more regional (far field) scale and for longer time periods. Model conceptualization is an abstraction process carried out by teams of experts. While using a consistent set of available site data and supplementary information, the different research groups are likely to obtain conceptual models that are different from and potentially inconsistent with each other. Evaluating these different conceptual models provides valuable insights into the system understanding and related uncertainties.

The main objective of this section is a comparative assessment of the different geosphere conceptualizations and modelling approaches used by the research teams to understand and predict the far field behaviour of a geological repository based on radionuclide transport simulations.

The comparison is performed for the following variants of the far field zone conceptual model:

- An equivalent porous medium model (CPR, LIT, ROM, UKR);
- An equivalent porous medium model with a discrete fracture (ROM, UKR) or a simplified discrete fracture model (CPR);
- A fracture network model (ROK).

To perform the analysis, the characteristic case results were taken for groundwater flow and transport modelling. As a conservative (non-sorbing) tracer, ^{129}I was chosen to analyse its possible migration from the deep geological repository into the groundwater discharge locations (river and well) in the upper aquifer of the modelled groundwater system. The following characteristic modelling results have been compared:

- Time plots of cumulative release into the biosphere (by CPR, LIT, and UKR data) normalized by total radionuclide activity in the container and starting time of release;
- Breakthrough curves to the discharge points expressed in relative concentration units (ROM) or in radionuclide flux units (ROK);
- Spatial distribution of the contaminant concentration plumes (LIT, ROM, UKR) and contaminant travel times from the repository to the discharge points.

This comparison study was performed by UKR based on contributions from LIT, CPR, and ROK.

4.3.2. Case description

4.3.2.1. General far field characteristics

The numerical models developed by CPR accounted for the hydrogeological characteristics of the semi-generic Veresnia site, Ukraine (see Annex I).

To study the groundwater flow regime in the far field zone around the repository and possible radionuclide migration from the repository, most teams developed a 2D (vertical cross section) flow and transport model with a layered hydraulic conductivity structure. The ROK team developed a 3D model, and CPR developed a 1D model.

The dimensions of the model section are 5000 m in the horizontal direction (from the repository location to the nearest river) and 1500 m in vertical direction (depth from the earth's surface). The repository location was defined to be on the left side of the model at a depth of 800 m. The river location was set on the right upper corner of the section, and the well location was defined on the top boundary at a distance of 3000 m from the repository.

Generally, all modelling teams used the same number of layers in the far field zone model, and the same or very similar data for hydraulic conductivity and porosity of these layers.

At the left and right vertical boundaries of the model section, a "no-flow" boundary condition is imposed with zero groundwater flow in the horizontal direction, except for the block representing the river, located at the upper right corner of the model, in which a constant head boundary condition was applied.

LIT, ROM, and UKR completed several simulation variants for fixed groundwater head in the river (-3 m) and variable drawdown in the well (from -3 to -6 m). For this comparison study, the variants were taken in which the prescribed head in the river and well were equal to -3 m.

A constant infiltration of 100 mm/y was defined at the upper model aquifer as groundwater recharge. This rate is based an assessment of the average annual precipitation, surface runoff and evaporation for the study area.

To make the results of different teams comparable, the differences in radionuclide release scenarios (release start time, number of defect canisters, radionuclide inventory) were removed by using release plots that are normalized by the radionuclide inventory and release start time. However, CPR, LIT, ROK, and UKR used the release scenario of a single defect canister containing 3.2 mol ^{129}I, and ROM assumed a simultaneous failure of all canisters in the repository (total inventory of ^{129}I is around 4500 mol). CPR, LIT, ROK, and UKR simulated the release duration of 10^6 years, whereas ROM assumed 10^4 years.

In the next few subsections, specific assumptions and conceptualizations about the far field made by the different modelling teams have been presented. The specifics include the type of model, its dimensions and discretization method, the simulation codes and calculation algorithms, as well as the inclusion of processes that determine the radionuclide transport.

4.3.2.2. CPR

Type of model, dimensions, and characteristics: The conceptual model of the far field geological medium was a 1D fracture zone (priority channel) embedded in a porous matrix of low permeability. Darcy's law and steady-state flow were assumed.

Codes, algorithms, processes: The GoldSim simulator was used. The software provides a graphical object-oriented environment for model construction and solution for a wide variety of problems. Algebraic equations, lookup tables, and dynamically linked process models can be used in a deterministic and stochastic (Monte Carlo) mode. CPR constructed a radionuclide transport model for ^{129}I and ^{79}Se, which includes both the near field and far field repository zones. Mathematically, the radionuclide transport model in the far field zone was represented by a 1D initial-boundary problem for a simplified channel aquifer (porous medium) with a single fracture (preferential flow channel). Advection, dispersion, and equilibrium sorption processes were taken into account. The problem was solved both in deterministic (finite difference) and stochastic (Monte Carlo) formulations. The values of the parameters in the far field (flow rate, fracture dimensions, porosity in the matrix and fracture) were taken from an SKB report [13] and the report by the LIT team [14]. For the stochastic modelling approach, the parameter ranges (min, max, and medium values) for each parameter have been assigned.

Data source: [15].

4.3.2.3. LIT

Type of model, dimension, and characteristics: A 2D flow and transport model and an equivalent porous medium (EPM) approach were used for the far field modelling. The domain was discretized into a mesh having 4100 quadrilateral elements (100 elements in horizontal direction and 41 elements in vertical direction).

Codes, algorithms, and processes: Flow and transport predictions were made using the TOUGH2 simulator [16]. It is a general-purpose numerical simulation program for multi-dimensional fluid and heat flows of multiphase, multicomponent fluid mixtures in porous and fractured media. It uses space discretization constructed directly from the integral form of the basic conservation equations, without converting them into partial differential equations.

The far field zone model constructed by LIT accounts for advection, dispersion, and equilibrium sorption. The model geometry and parameters (hydraulic conductivities, porosities) are taken close to ones taken by UKR.

Data source: [11].

4.3.2.4. ROK

Type of model, dimensions, and characteristics: A 3D discrete fracture network (DFN) model for the Veresnia site (Fig. 6) has been developed [17]. The model section length was increased by 1500 m on the left side from the repository location, and the section depth at the new left model boundary was increased to 1650 m with a no-flow boundary condition. The model width was taken to be 1500 m.

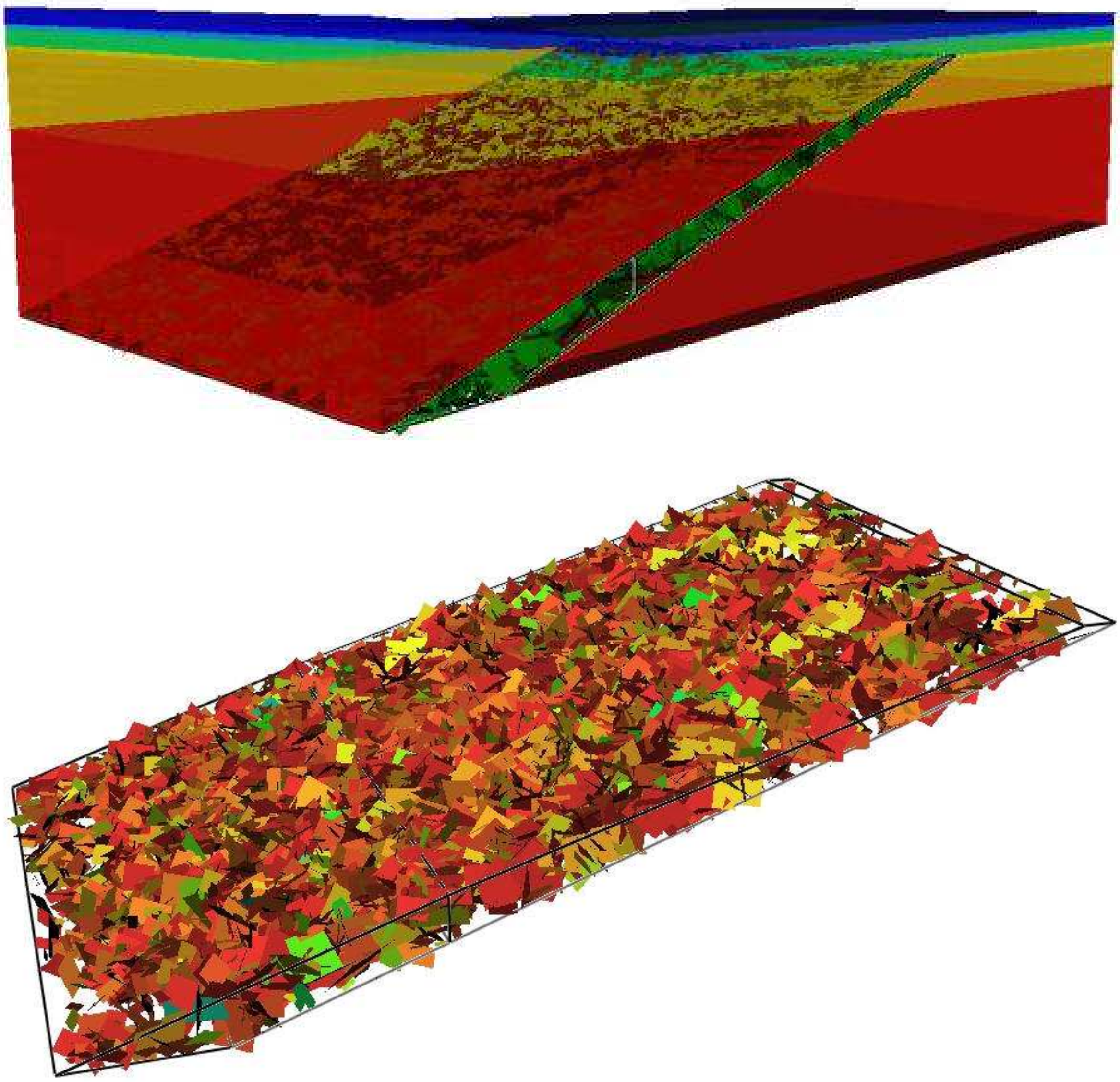


FIG. 6. Three-dimensional discrete fracture network (DFN) model of the Veresnia site.

Codes, algorithms, and processes: The codes ConnectFlow [18] and Mascot-K [19] were used. The ConnectFlow (CONtinuum and NEtwork Contaminant Transport and FLOW) code by Serco Assurance Ltd. is a software package for modelling 3D groundwater flow and transport in porous and fractured media. It is based on two submodels: NAMMU [20], for solving the standard advection-dispersion-sorption partial differential equations in a continuum porous medium, and NAPSAC [21], for simulating a discrete fracture network using a particle-tracking algorithm. ConnectFlow provides all of the functionality of the original finite-element codes NAMMU and NAPSAC designed by AEA Technology and combines these functionalities in a complex porous-fracture model. The MASCOT-K probabilistic safety assessment code was designed by KAERI [19, 22] based on the original MASCOT code [23] designed by SERCO (UK). Each module corresponds to a specific process or barrier and evaluates the corresponding analytical solutions. Unlike the original MASCOT, the MASCOT-K is able to also simulate the SNF dissolution mechanisms. It predicts flux and contaminant concentration at a given time and position.

The far field zone simulation is based on the fractured geosphere and porous geosphere sub-modules. The fracture sub-module examines radionuclide migration along a straight fracture, taking into account advection, dispersion, sorption, kinetic reactions and matrix diffusion. The porous geosphere module uses the equivalent porous medium (EPM) model.

The normalized accumulative release curves for the comparison study were obtained based on radionuclide release curves.

Data source: Ref. [17].

4.3.2.5. ROM

Type of model, dimensions, and characteristics: A 2D flow and transport model and an EPM approach were used for the far field modelling. In addition, the effect of an inclined fault was considered. The fault was modelled as an individual fracture (with different aperture) passing through the repository and ascending in the direction of the internal discharge boundary (well).

Codes, algorithms, and processes: The finite element code FEFLOW 5.2 (by WASY GmbH) was used for the simulations. The domain was discretized into 70216 triangular elements and 35736 nodes; the length of an element side was about 9.0 m. The upper limit of the time step was 10 years. Advection, dispersion, and equilibrium sorption processes were taken into account.

Data source: Ref. [24].

4.3.2.6. UKR

Type of model, dimensions, and characteristics: A 2D flow and transport model and an EPM approach were used for the far field modelling. A variant of the model includes a discrete inclined fracture zone, allowing for a potential fast-flow pathway from the repository to shallow aquifers and the internal discharge boundary (well). The discretization grid of the domain has 9 layers in depth and 100 blocks in the horizontal direction.

Codes, algorithms, and processes: The model was developed using the 3D Processing MODFLOW (Ver. 5.3) hydrogeological modelling system [9]. The system is based on the MODFLOW code [25] for groundwater flow, and MT3D/MT3DMS codes [26, 27] for contaminant transport. Advective transport paths and transport times were evaluated using the particle tracking method [9, 28], realized in the code PMPath by successive execution of MODFLOW and PMPath for each simulation variant. Advection, dispersion, and equilibrium sorption processes were taken into account for modelling radionuclide transport. For comparison purposes (case ^{129}I), only the modelling variants with advection were considered.

Data source: Ref. [29].

4.3.3. Simulation results

For the comparison study, the releases of ^{129}I into the well and river have been calculated and corresponding time plots were created by the teams of LIT, ROK, CPR and UKR.

The simulation results can be grouped in the following way:

- Different types of the far field conceptual model: equivalent porous medium (EPM) and discrete fracture network (DFN) models;
- Different codes and dimensions of far field EPM models;
- Different approaches and dimensions of fracture zone models.

Besides this, additional information about contaminant particle path lines and travel time to discharge zones are used for the comparison study.

The results of the comparative analysis are discussed in the following sections according to these groups.

4.3.4. Comparative analysis

4.3.4.1. Different types of conceptual far field model

The normalized cumulative release plots calculated for ^{129}I using EPM and DFN models are shown in Fig. 7. It is seen from the figure that:

- Both types of far field model give comparable results of cumulative release (within one order of magnitude), if the time period of the integral assessment approaches 1 million years;
- The DFN model predicts an early breakthrough of ^{129}I into the river, with cumulative release exceeding 10^{-5} at 10^3 years after ^{129}I outflow from the repository; the release rate becomes approximately constant at time 10^4 years;
- For the EPM models, the cumulative release of ^{129}I into the river exceeds 10^{-5} after $3 \cdot 10^5$ years (LIT), and after $4.5 \cdot 10^5$ years (UKR), and the release rate approximates a constant after 10^6 years (for both cases).

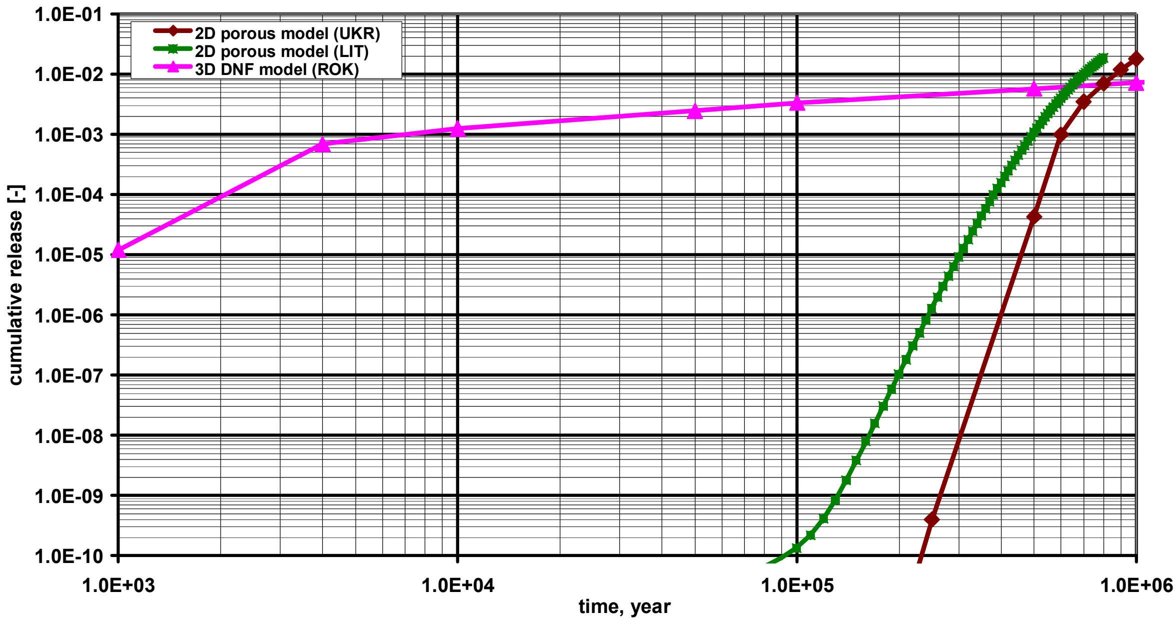


FIG.7. Normalized cumulative release of ^{129}I into the river for the EPM and DFN geosphere models.

4.3.4.2. EPM models of far field zone using different codes and model dimensions

The normalized cumulative ^{129}I release curves calculated for different variants of the EPM models are shown in Fig. 8.

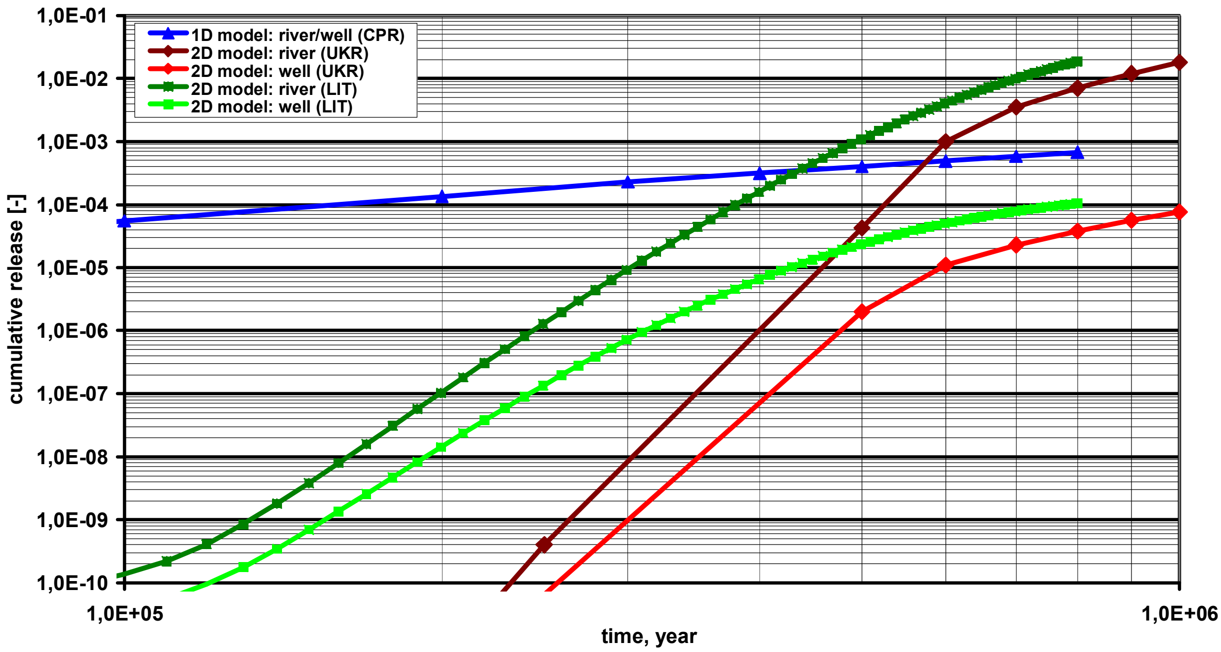


FIG. 8. Normalized cumulative ^{129}I release into the river and well for the EPM geosphere models.

Predictions of cumulative release using different codes and model dimensions, but a consistent EPM geosphere models are overall in good agreement:

- The normalized ^{129}I cumulative release curves for obtained by LIT and UKR converge as the time approaches 1 million years;
- The difference between releases into the river and well are approximately the same given data of LIT and UKR. The differences are about 1 order of magnitude after 300 000 to 400 000 years and close to two orders of magnitude after 10^6 years. Similarly, the difference of the maximum ^{129}I concentrations at the river and the well comprises about 1.5 orders of magnitude according to the ROM simulation results reported in Ref. [24];
- The curve obtained by CPR looks like an average of the LIT and UKR release curves. Note that the 1D conceptualization does not distinguish between releases to the river and the well.

The main difference between the results consist in the observed "time shift" between the release curves. As compared with CPR model, the same release values are achieved after:

- $4.2 \cdot 10^5$ years for the LIT model;
- $5.7 \cdot 10^5$ years for the UKR model.

4.3.4.3. Fracture zone models

The calculation results for normalized ^{129}I cumulative release for different fracture zone models are shown in Fig. 9.

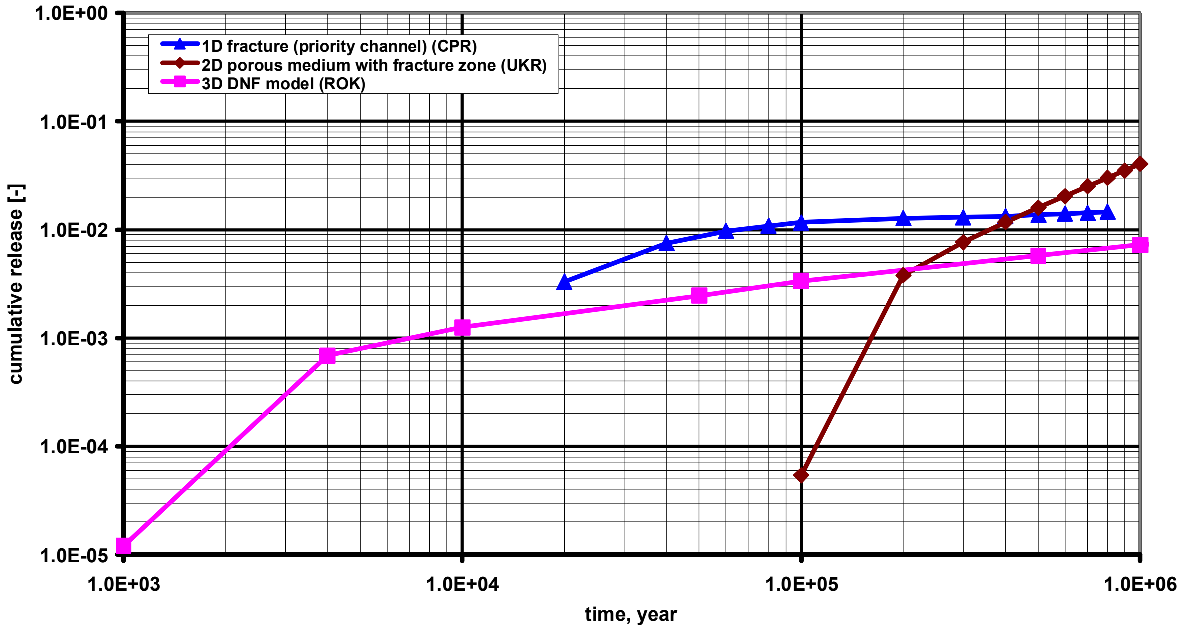


FIG. 9. Normalized cumulative release of ^{129}I from the far field zone for different fracture zone models.

The figure shows that:

- CPR and ROK give comparable assessments of the cumulative release (within one order of magnitude);

- The results of UKR differ in that release to the river starts later and reached a higher value.

4.3.4.4. Additional data

The information about the contaminant pathway length and its travel time to the discharge points obtained by different far field models is given in Table 1.

TABLE 1. CONTAMINANT PATHWAY LENGTH AND TRAVEL TIME TO DISCHARGE POINTS FOR DIFFERENT FAR FIELD ZONE MODELS

Country	Type of geosphere conceptualization	Contaminant pathway length (m)	Travel time (y)	Comment
CPR	1D Priority channel	5500	Approx. 100 000	According to ^{129}I steady flux
LIT $H_r=H_w=-3$m	2D EPM		More than 800 000	According to ^{129}I steady flux
UKR $H_r=H_w=-3$m	2D EPM	7100	1 350 000 (particle tracking method)	Length of path and travel time strongly depends on heads at the discharge points
	2D EPM + fracture zone		1 200 000 (particle tracking method) 100 000 (steady concentration of ^{129}I at the discharge points)	
ROM $H_r=H_w=-3$m	2D EPM		Approx. 180 000	According to ^{129}I maximal concentration
	2D EPM + fracture with aperture 0.1 mm	3230	Approx. 80 000	According to ^{129}I steady concentration
	2D EPM + fracture with aperture 1.0 mm		Approx. 1800	
ROK	3D DNF	5120	842	

The data given in the table shows that:

- The travel time assessments differ significantly for different geosphere models (by 2-3 orders of magnitude) as well as within a given model (by 1 order of magnitude);
- The fracture zone modelling based on the EPM approach gives longer travel times to discharge points as compared to the DFN approach;

- The particle tracking method gives travel times to discharge points which do not agree with assessments that are based on reaching a steady-state concentration.

The particle tracking method as implemented in the code PMPath [28, 30] which is part of the PMWIN [9] package, was used to analyse the general flow pattern, the main contaminant transport directions and corresponding travel times. The particle tracking method accounts for advective transport of radionuclides through the effectively available pore space; retardation due to sorption is also included. Dispersion is not taken into account, which may partly explain the differences to the results obtained with other transport simulation methods. The pure advection solution in most cases appears to be more conservative, because it does not lead to the splitting and branching of path lines as described by the dispersivity of the medium.

The comparison of the EPM geosphere models shows that:

- The contaminant pathway length calculated by CPR is shorter than the more complicated pathways obtained by UKR and LIT with Darcy velocity along the horizontal sections of the pathways being higher than along vertical sections. CPR used the velocity assessment from horizontal pathway sections. This explains the earlier breakthrough obtained by CPR;
- UKR did not account for dispersion in the model variants used for ^{129}I release calculations. For this reason, curves obtained by UKR show a time delay compared to those obtained by LIT;
- Different codes used by different teams provide comparable values of the entire release curve.

4.3.5. Conclusions

EPM versus DFN approach: The EPM approach appears appropriate for modelling of steady-state processes and for sedimentary rocks. The EPM model gives smoother distributions of the contaminant concentrations and higher contaminant travel times than the DFN model. The EPM model provides better reflection of the space distributed barrier properties of the sedimentary rocks (and maybe fringe fractured zone of the base rocks), especially in case of relatively high distribution coefficients (or retardation factors) for these deposit types and radionuclides. These features of the EPM provide for a more optimistic repository safety assessment, and in case of insufficient data, the non-conservative nature of the forecast must be considered. The DFN model does not produce a diffusive behaviour expected in a porous-medium type geological environment, but highlights discrete flow and transport behaviour in a fractured or dual-porosity medium. This generally results in shorter travel times and correspondingly more conservative repository safety assessments. This model is more appropriate for fractured host rocks with known types of fracturing and characteristic fracture network dimensions.

The model of a single inclined fracture zone used by UKR is a rather conservative assessment for the specific case of a macro-fracture zone (tectonic break) that has a length comparable with the model size. The model gives comparatively high contaminant concentrations and low travel times in the case of zero or low sorption (e.g. for ^{129}I), complicated contaminant particle pathways (especially in the case of equal well and river drawdowns of -3 m, which causes an unstable stagnation zone with discharge directions either to the river or the well, with corresponding increases of travel times), and significant Darcy velocity differences along the migration pathway.

The discretization type (finite difference, finite elements) and *degree of resolution* (finer grid) are essential for parametric data with higher spatial dimensions. For the general case of relatively homogeneous data for hydraulic conductivities and porosities in the horizontal plane, the different discretization types and mesh sizes used by the different teams do not cause significant differences in the results (contaminant plume geometry, ratio of releases into the river and well, etc.).

The influence of model dimensionality (1D, 2D, and 3D) leads to differences in the cumulative release values of approximately one order of magnitude. Such a difference is not very significant given the high uncertainty of the initial data and the different modelling approaches used by the teams participating in this comparison study. However, the differences in contaminant travel times and releases at early times are greater, especially between the 1D model and 2D/3D models.

Different codes give comparable release values for the EPM model. However, the difference in travel times is more significant, which is most likely attributable to other differences in the model approaches (dimension, discretization, etc.).

Restrictions of analysis: The country cases considered differ in conceptualization, assumptions, parameters, and simulation tools. This makes it difficult to separate and assess the comparative influence of an individual parameter or feature on the results.

4.4. IMPACT OF USING PROCESS MODEL OR TSPA APPROACHES

4.4.1. Objectives

The purposes of evaluation of process model and TSPA approaches are to (1) understand the process of performance assessment of a geological repository on the system level, (2) review the differences in results obtained by different models and approaches, (3) understand the advantages and disadvantages of numerical modelling, and (4) gain expertise in using different process model and performance assessment codes. The main objective is a comparative analysis of process model and TSPA approaches for the assessment of the engineered and natural barriers of a geological repository for the disposal high level nuclear waste.

This comparison study is carried out by CPR with contributions from UKR and ROM.

4.4.2. Case description

The comparison is done for the following processes and conceptual model:

- Release of radionuclides from waste form, and its transport driven by hydraulic and concentrate gradient through backfill barrier to the EDZ, to the water-bearing formation, and finally to a river or well;
- Disposal concept: near field model of KBS-3; far field model of Ukrainian semi-generic site;
- Geosphere model: Equivalent porous medium (CPR, ROM, UKR);
- Alternative geosphere model: Equivalent porous medium with discrete fracture (ROM, UKR) or a discrete fracture (CPR).

Different codes were used to perform the simulations. GoldSim was used by CPR, PMWIN by UKR, and DUST-MS and PORFLOW by ROM for the simulation in the near field and far field, respectively.

4.4.2.1. Characteristics of geological disposal system

The geological disposal system consists of a near field and far field subsystem. The teams participating in this comparative analysis used the same conceptual model of the repository system. The near field model is based on the KBS-3 concept, and the far field model is based on the UKR semi-generic site (see Annex I).

The following subsections describe the differences among the models, such as the type of model, its dimensions and discretization method, codes and calculation algorithms.

4.4.2.2. Description of CPR model

Type of model, dimensions, and characteristics: The system-level model developed by CPR simulates the multi-barrier system of geological disposal by integrating both the near and far field. The near field model, which is similar to that developed by LIT, has been divided into nine model blocks, two water blocks representing the void inside the canister and the hole through the canister wall, four blocks representing the bentonite, two blocks representing the crushed rock-bentonite and one for the rock below the deposition hole. Some blocks are further divided for a total of 19 compartments in the model. The discretization of the near field is presented in Fig. 2(b) and reproduced here in Fig. 10. The radionuclide transport driven by the hydraulic gradient in the near field is the same as that in the far field.

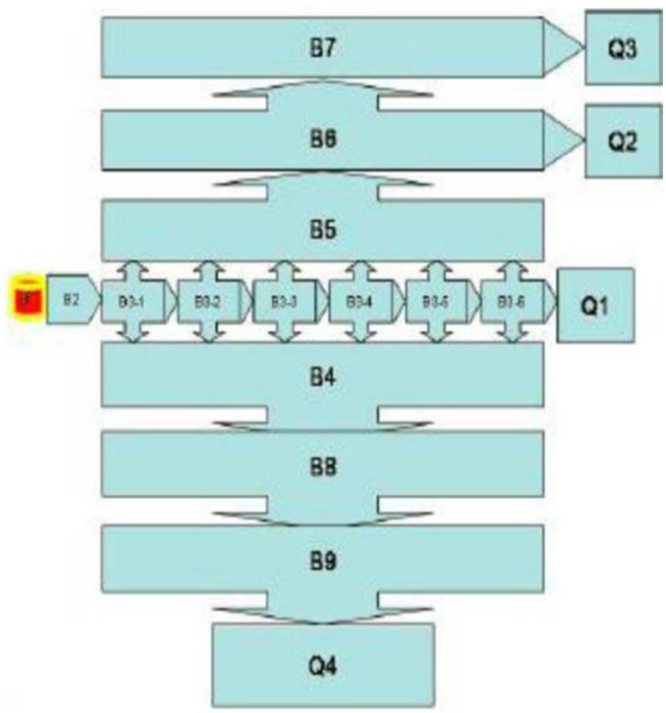


FIG. 10. Simplified near field model.

The far field model is a simplified, one-dimensional representation of the semi-generic Veresnia site described in Annex I. Unlike the models developed by UKR and ROM, the CPR conceptual model of the far field includes a 1D fracture zone (priority channel) embedded in a porous matrix of low permeability (Fig. 11). Steady-state flow according to Darcy's law is assumed.

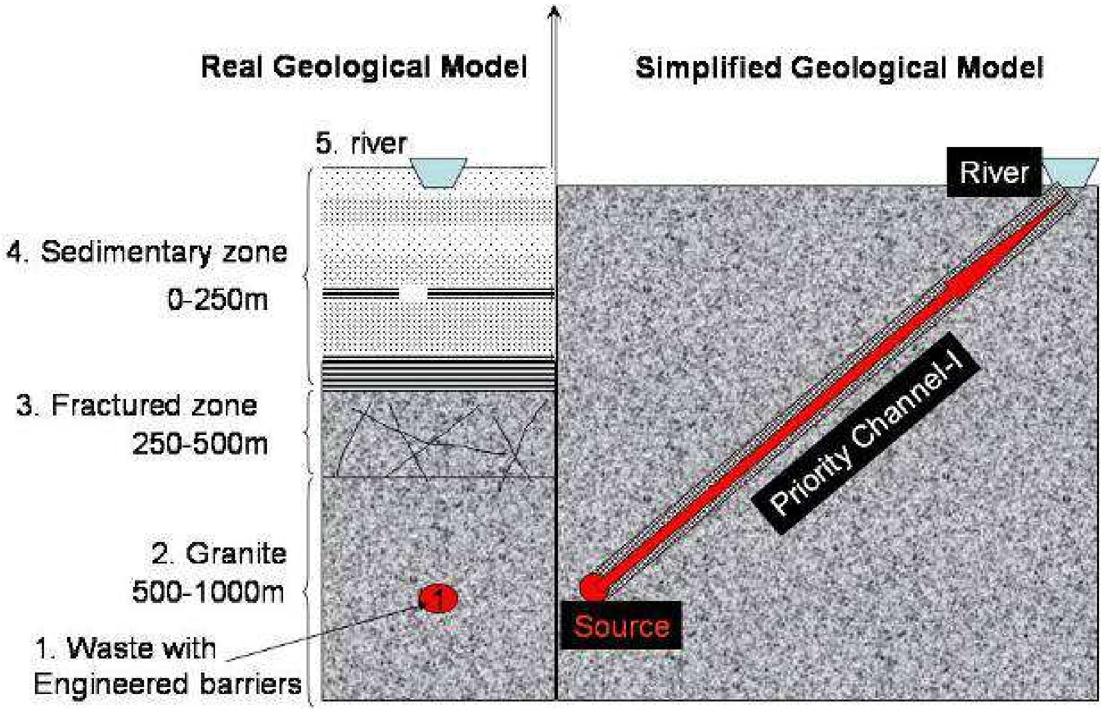


FIG. 11. Simplified one-dimensional representation of the geological disposal system.

Codes, algorithms, and processes: The GoldSim system-level code was used for the simulation of the transport of ^{129}I and ^{79}Se in both the near field and far field repository zones. Advection, dispersion, and equilibrium sorption processes were taken into account. The problem was solved both in deterministic and stochastic (Monte Carlo) formulations. In the deterministic calculation, the parameter values in the near field are the same as those used by ROM. However, the parameter values (flow rate, fracture dimensions, porosity in the matrix and fracture) of the far field are different from those used by other teams. In the stochastic analysis, parameter ranges (min, max, and mean values) for each parameter were assigned.

Data source: Ref. [15].

4.4.2.3. Description of ROM model

Type of model, dimensions, and characteristics: The near field conceptual model developed by ROM differs from that developed by LIT and used by CPR. ROM used the Canadian disposal concept (CANDU spent fuel). The model is described in Annex VI. The ROM model also considers the influence of temperature and gas generation on the release of radionuclides from the near field.

A 2D flow and transport model and an equivalent porous medium (EPM) approach were used for the far field modelling. The fault was modelled as an individual fracture (with different aperture) passing through the repository and ascending in the direction of the internal discharge boundary (well).

Codes, algorithms, and processes: DUST-MS and PORFLOW were used by ROM for the simulation of the near field and far field, respectively.

Data source: Ref. [31].

4.4.2.4. Description of UKR model

Type of model, dimensions, and characteristics: A 2D flow and transport model and an EPM approach were used for the far field modelling. A variant of the model includes a discrete inclined fracture zone, allowing for a potential fast-flow pathway from the repository to shallow aquifers and the internal discharge boundary (well). The discretization grid of the domain has 9 layers in depth and 100 blocks in the horizontal direction.

Codes, algorithms, and processes: The model was developed using the 3D Processing MODFLOW hydrogeological modelling system [10]. The system is based on the MODFLOW code for groundwater flow [22], and the transport code MT3DMS. Advective transport paths and transport times were evaluated using the particle tracking method [10, 30] realized in the PMPath code by successive execution of MODFLOW and PMPath for each simulation variant. Advection, dispersion, and equilibrium sorption processes were taken into account. For the comparison study, only advection of ^{129}I was considered.

Data source: Ref. [32].

4.4.3. Simulation Results

4.4.3.1. Deterministic simulations

The transport of two radionuclides (^{129}I and ^{79}Se) through the near and far fields to the river and well is calculated using GoldSim. Figs 12 and 13 show the normalized cumulative activity (which is defined as the cumulative activity in the river/well divided by initial activity in the canister) released from the near field and discharged to the river for both the fracture zone and surrounding matrix.

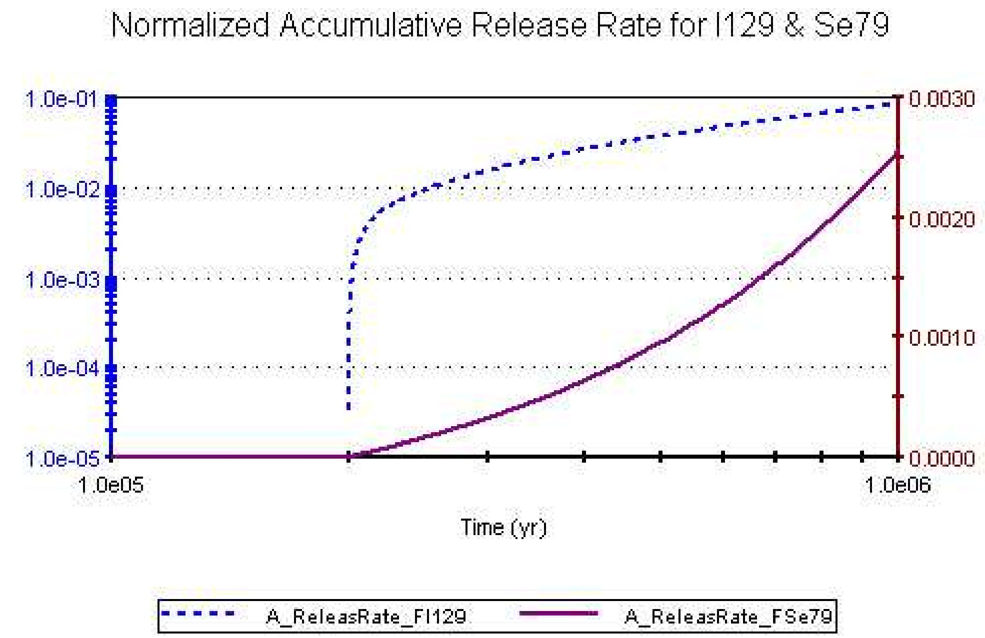


FIG.12. Normalized cumulative release rate through fracture zone to river and well.

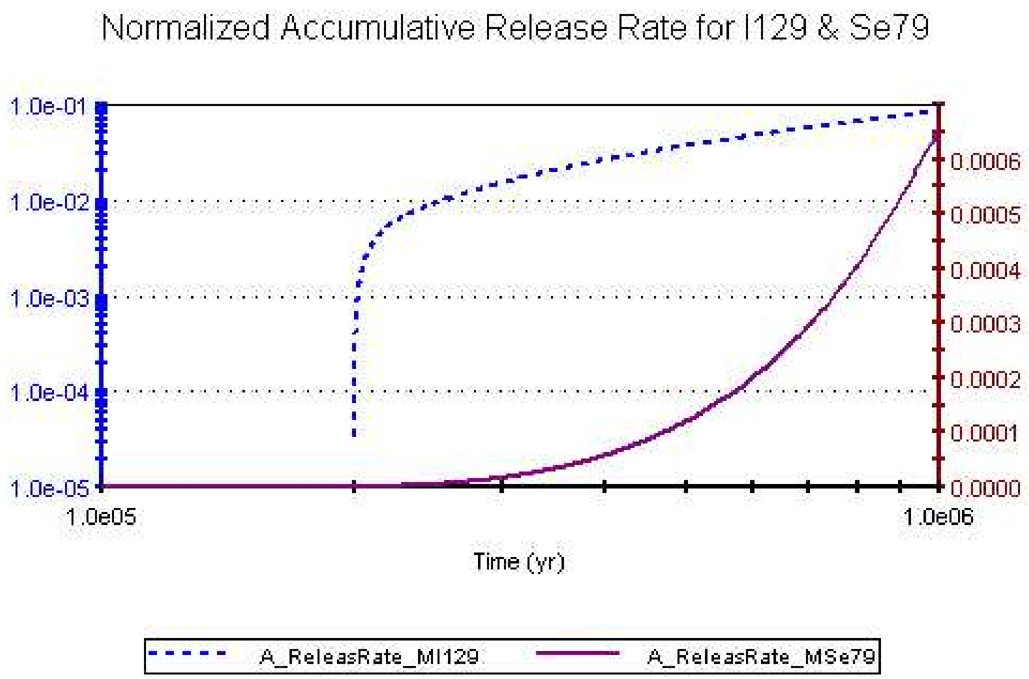


FIG. 13. Normalized cumulative release rate through matrix to river and well.

4.4.3.2. Probabilistic simulations

In the probabilistic simulations of the transport of ^{129}I and ^{79}Se, the following six parameters are considered uncertain: Instant release fraction (IRF), solubility, porosity, sorption, geometry of the fracture domain, and water flowrate. Uncertainty distributions were defined for these six parameters, and 50 Monte Carlo realizations were examined to a simulation time of 1 million years. The results are shown in Figs 14 to 17.

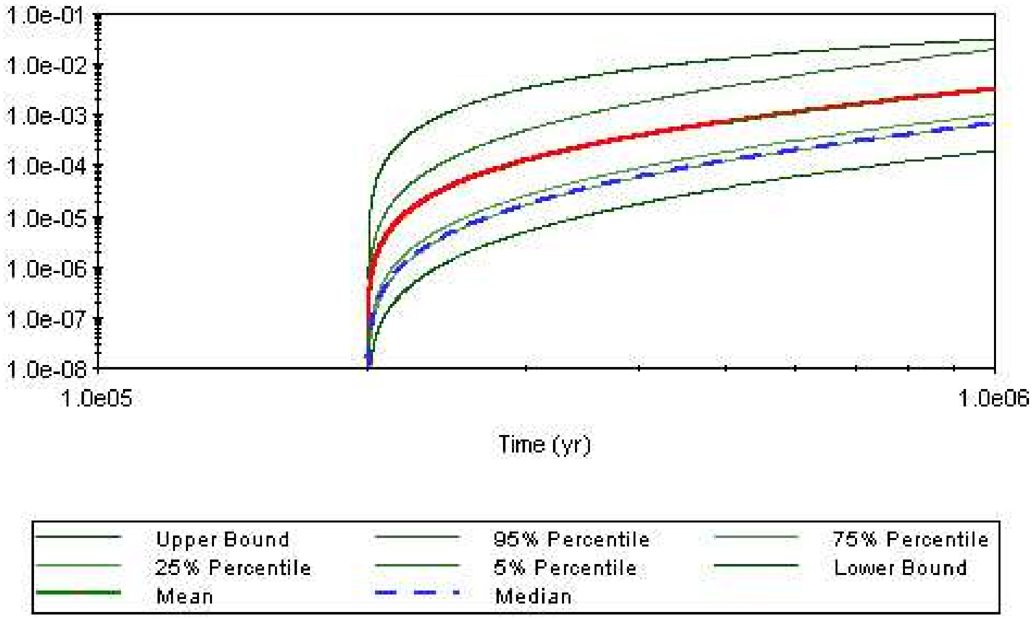


FIG.14. Probabilistic cumulative release rate curves for ^{79}Se in matrix.

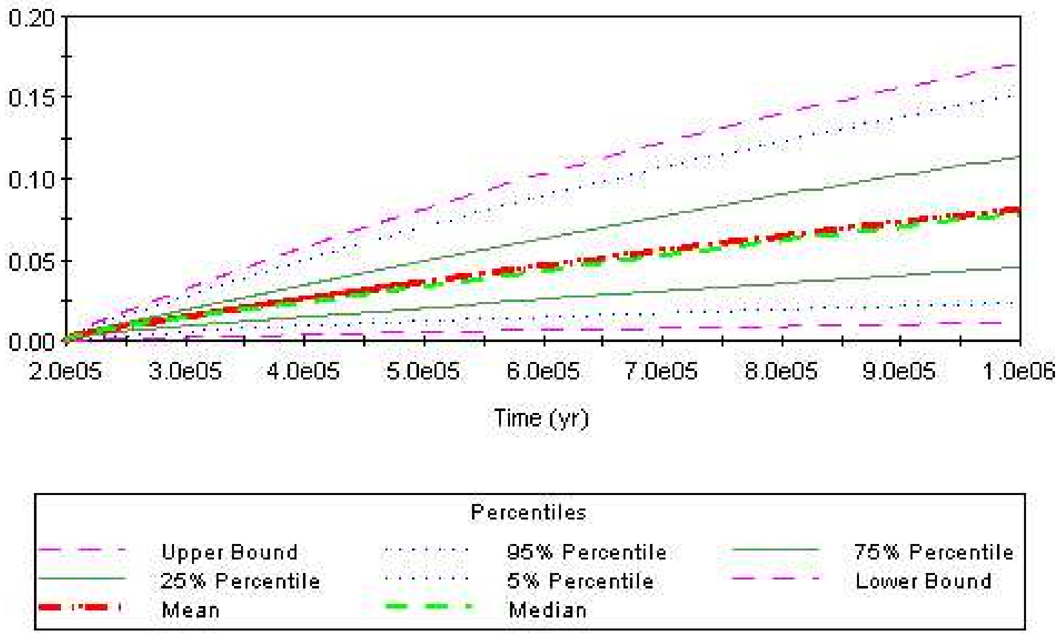


FIG. 15. Probabilistic cumulative release rate curves for ^{129}I in matrix.

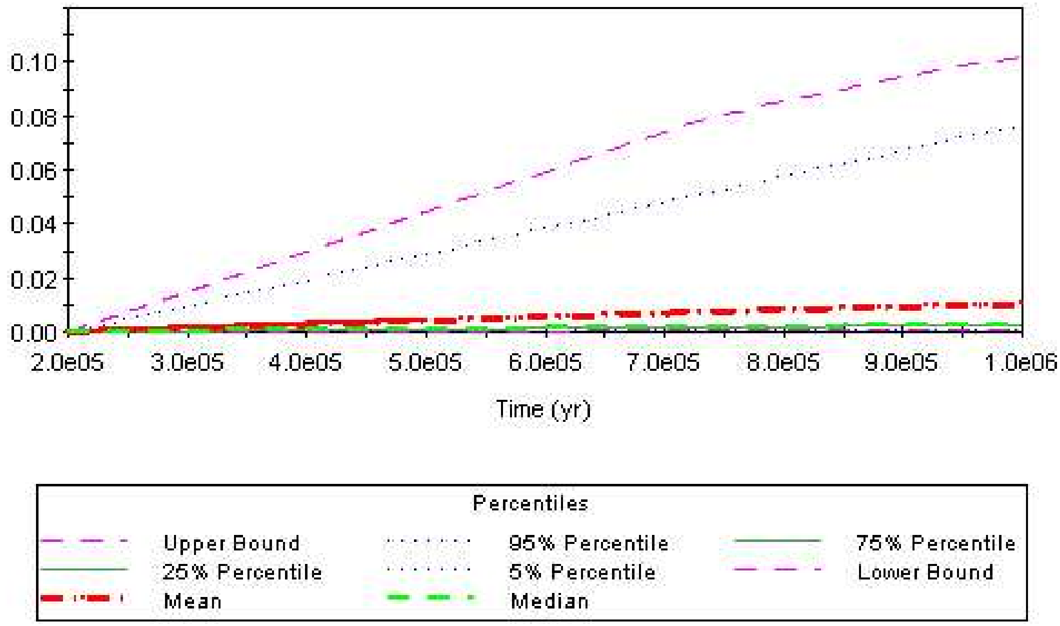


FIG. 16. Probabilistic cumulative release rate curves for ^{79}Se in the fracture domain.

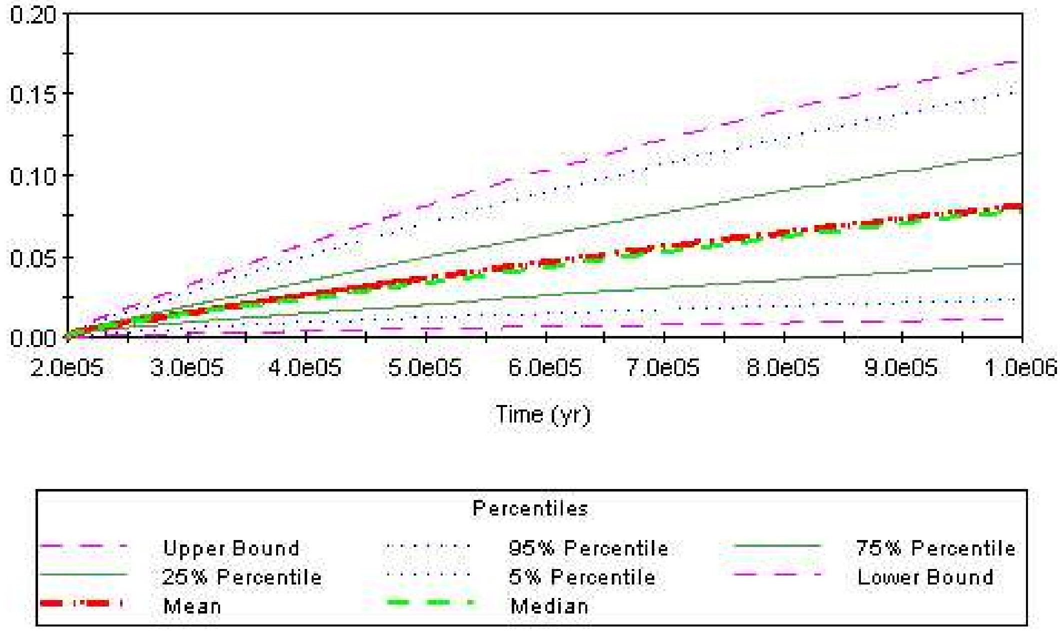


FIG. 17. Probabilistic cumulative release rate curves for ^{129}I in the facture.

4.4.4. Comparative analysis

The comparative analysis considers the migration of ^{129}I from the waste canisters through the geosphere to the groundwater discharge locations (river and well) in the upper aquifer. The cumulative release into the biosphere normalized by total radionuclide activity is used as the result to be compared.

4.4.4.1. Comparative analysis CPR and ROM

The results obtained from CPR and ROM are shown in Figs 18 and 19 respectively.

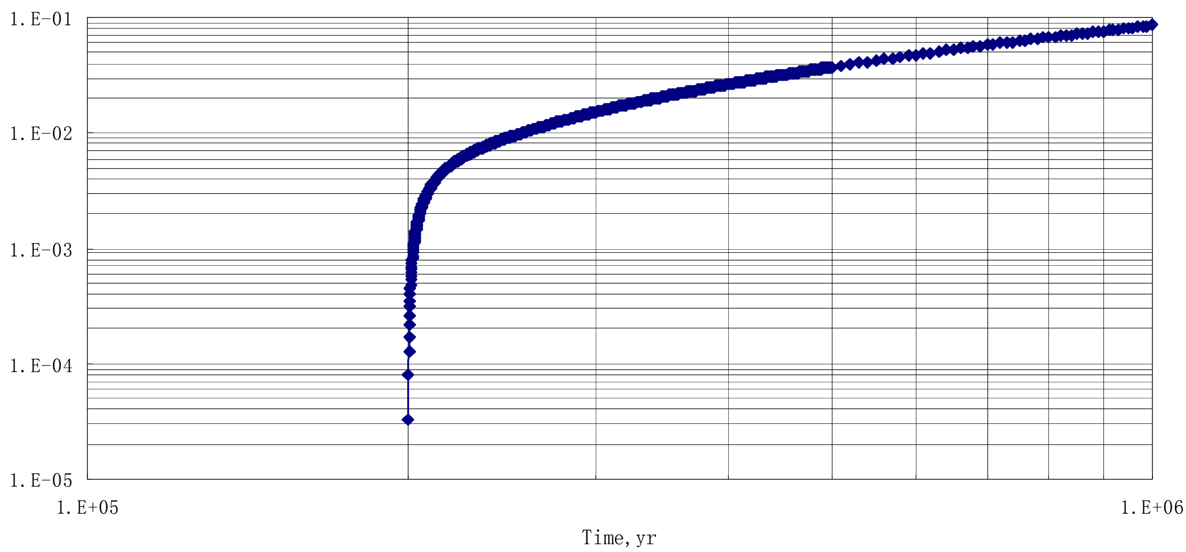
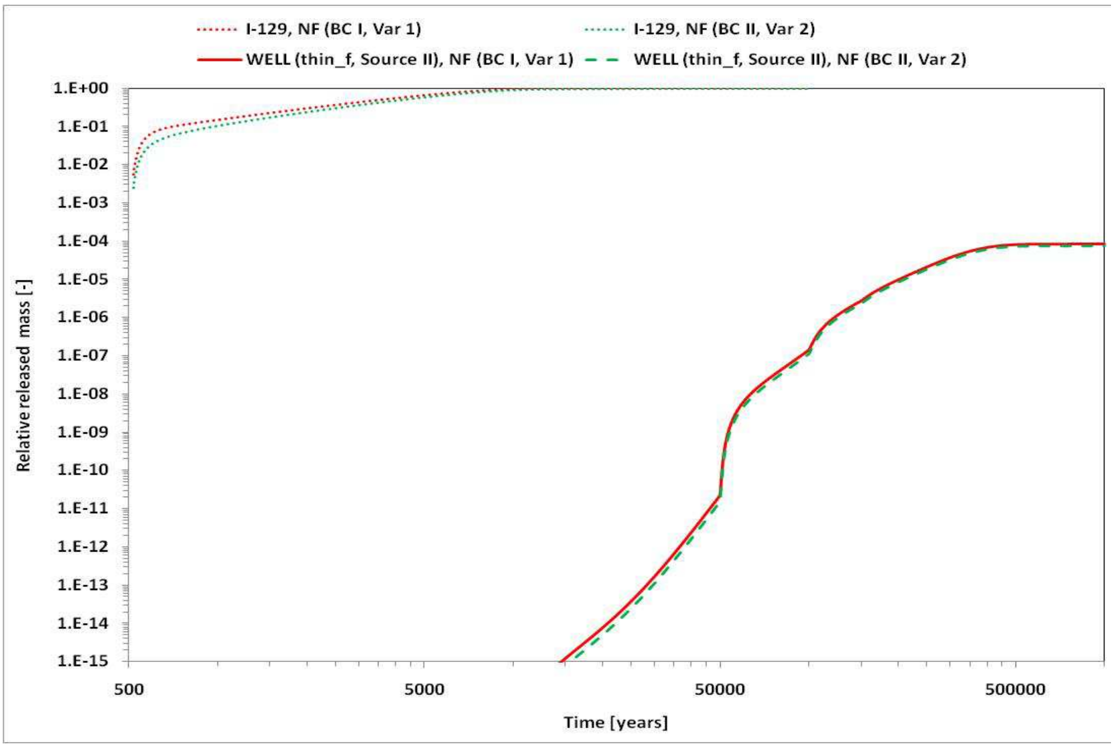
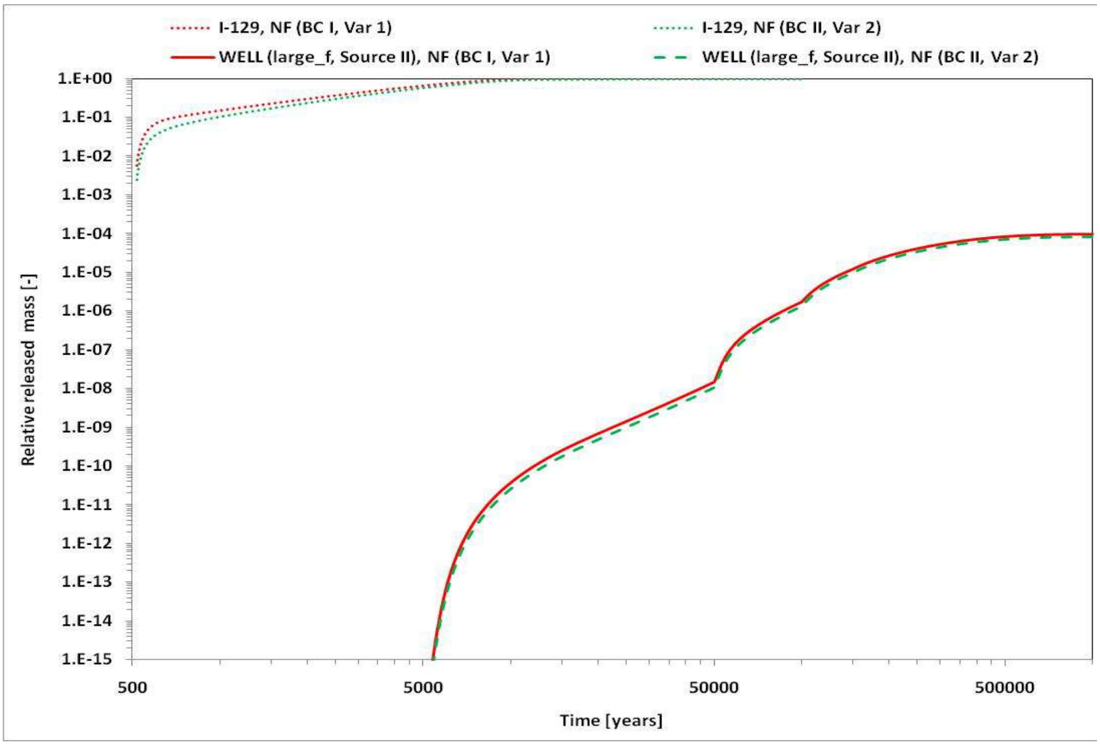


FIG. 18. Normalized cumulative release rate curves for ^{129}I at the well through fracture, calculated by CPR.



(a) fracture aperture: 0.1 mm.



(b) Fracture aperture: 1.0 mm.

FIG. 19. Relative released mass of ^{129}I for different types of boundary conditions at the buffer outlet. Near field released mass for zero concentration boundary conditions at the buffer-rock interface (BC I, Var 1) and zero flux at a symmetry boundary (50 times buffer width) (BC II, Var 2).

4.4.4.2. *Comparative analysis CPR and UKR*

The differences between CPR's and UKR's results are described in detail in Section 4.3.4. Potential causes of the differences include:

(1) Different assumptions underlying the far field model: 1D for CPR and 2D for UKR. The 2D results are considered more realistic than the 1D results;
(2) CPR integrated the engineered barrier sub-system and natural barrier sub-system of geological disposal by using the same hydraulic gradient, whereas in UKR's conceptual model, the geological disposal system was divided into two parts, where the releases from the engineered barrier system are implemented as a source term or initial condition of water flow and solute transport in the far field model. The GoldSim TSPA approach is considered more realistic in this regard;
(3) During calculation, steady-state flow is assumed by GoldSim code;
(4) There are many factors having influence on the water flow and radionuclide migration in the total system of geological disposal, including the initial conditions and boundary conditions, instant release fraction (IRF), solubility, porosity and sorption, geometry of fracture domain and so on. GoldSim uses Monte Carlo method to do the probabilistic simulation and the effect of coupling of multi-factor interaction can be obtained by GoldSim but the other codes perhaps only assess the impact of initial and boundary conditions.

4.4.5. Conclusions

The following insights were gained through the simulation and comparison analyses performed as part of this project:

(1) *Understanding of difference between process model and TSPA approach*: The purpose of process modelling is to appropriately simulate the advective and dispersive transport of radionuclide along a fracture and their diffusion and retardation in the matrix. Once process understanding has been gained and key factors identified, a simplified model can be developed to study the behaviour of the entire system (near field and far field) in a probabilistic TSPA calculation;
(2) *Impact of model dimensionality*: Model dimensionality significantly affects simulation results. The choice of the appropriate model dimensionality depends on the dominant flow and transport mechanism, site geometry, and purpose of the modelling (e.g. whether realistic or conservative results are desired);
(3) *Advantages and limitations of simulation codes*: In this comparison study, results from the TSPA code GoldSim are compared to the process simulators DUST-MS, PORFLOW, FEFLOW, MODFLOW). The advantage of GoldSim is that probabilistic calculations can be performed using the entire repository system (near and far field). Conversely, the process models are more appropriate for properly including the geometry and geologic structure of the repository site. More realistic flow fields calculated by the process models could be used as input to the transport simulations by the TSPA model.

5. CONCLUDING REMARKS

The stated purpose of this five-year CRP on "*The Use of Numerical Models in Support of Site Characterization and Performance Assessment Studies of Geologic Repositories*" was to transfer modelling expertise to selected Member States in support of their national nuclear waste management programmes. The broad scope of the topic, the significant complexity inherent in numerical modelling, and the fact that country-specific interests and needs had to be considered, made the coordination of this CRP challenging from a technical perspective. The following concluding remarks intend to clarify the outcomes, to explain the management approach, and to summarize the achievements and lessons learned from this exercise.

5.1. GENERAL COMMENTS

- As stated in the overall goals (Section 1), the intent of this CRP was to expose the participants to a number of modelling issues relevant for a performance evaluation of a nuclear waste repository. Besides addressing technical modelling issues, emphasis was placed on the discussion of the fundamental model development process, stressing the importance of the conceptual model as the basis for any predictive simulation. Uncertainties in the conceptual model far outweigh the impact of parametric uncertainty and numerical inaccuracies—a fact that was also demonstrated by the results of the comparison studies performed as part of this CRP;
- Given the requirements to address fundamental issues and the nature of this CRP, which is to provide guidance, it must be recognized that the participants were *not* expected to develop models that will be potentially used as part of their country's licensing process;
- While the fundamental modelling concepts have general applicability, it was the declared intent of the CRP to acknowledge the specific interests of the participants in order to make the CRP project more relevant for their respective country's repository programme. This means that a variety of waste specifications, repository concepts, host rocks, release scenarios, overall repository settings, and characterisation data had to be considered. Moreover, the specific scientific interest and expertise of the participating researchers was respected. In an attempt to accommodate this diversity of issues and interests, it was decided to follow a two-pronged approach:
  - — A semi-generic site was described (Annex I) to provide a common basis for a set of model simulations that are dedicated input to four comparison studies (see Section 4). The purpose of the comparison studies was to obtain broader insights (leveraging on each participant's suite of simulations using different approaches) into model uncertainties, and to encourage collaboration and discussion;
  - — Specific simulation studies were performed that address country-specific issues of interest to the individual participants (see Section 3 and Appendices C–F). The purpose of this set of analyses was to address particular modelling issues in support of each country's waste disposal programme.
- Only a limited amount of site characterization data was available, which led to focus on the study of a semi-generic site. Furthermore, no exercises for data analysis, inverse modelling, or model validation were performed;
- The comparison analyses conducted as part of this CRP were not designed or intended to be benchmarks of computer codes. Most of the codes used by the participants have been previously verified, benchmarked, and cross-validated. The purpose of the comparison studies was to examine prediction uncertainties as a result of choosing alternative conceptual models, modelling approaches, and scenarios. This is consistent with the previously stated focus of this CRP;

- The scope and nature of this CRP required a substantial amount of coordination and collaboration among the participants. The three RCMs were essential to coordinate the activities and to make necessary adjustments (see Section 2). Based on very effective discussions during the RCMs and upon review of deliverables, an action plan was developed by IAEA to further guide the research. In between the RCMs, it was up to the participants to exchange information and collaborate on the comparison studies;
- The Scientific Coordinators play a useful role, providing technical expertise, defining objectives, and coordinating the activities. The number and roles of participants (Contract holder, Agreement holders, Scientific Coordinators) needs to be carefully balanced.

5.2. TECHNICAL CONCLUSIONS

- A relatively large number of simulations codes (see Annex III) were used by the participants to perform the simulation tasks of this CRP. The participants did not seem to encounter significant technical difficulties in running the simulators;
- The results of flow and radionuclide transport simulations were found to be largely independent of the particular software being used;
- Model predictions are highly sensitive to decisions about the model structure, the features implemented, and parameterization;
- Assumptions about the system behaviour (specifically regarding the failure scenario, waste dissolution process, leakage pathways, and location of and conditions at the compliance boundary) have a dominant impact on contaminant travel time and exposure dose;
- Simulation assumptions and results need to be carefully documented and presented in a consistent, traceable and reproducible manner to avoid ambiguities and misunderstandings. The reasonableness of simulation results must be carefully checked using independent information and cross-validation. A physical understanding of the system behaviour is essential, and unexpected simulation results must be justified and explained.

5.3. LESSONS LEARNED

- The decision to go beyond a mere benchmark exercise and instead to conduct a challenging comparison study to examine conceptual model uncertainty proved to be ambitious. First, the design of the comparison study was difficult given the large variety of possible simulation scenarios and the correspondingly limited overlap in cases considered by the four teams. Such overlap is needed for the comparison study to yield conclusive results. The four comparison studies developed during the RCMs—while of limited scope—had the potential to provide useful insights into the reliability of model predictions; this potential was only partly realized. The second challenge faced by the comparison study was the required high level of collaboration and coordination among the participants. Small meetings in between RCMs may help facilitate interactions among the participants;
- The background, specialization, and level of expertise in numerical modelling varied considerably among the participants. This CRP benefited from the supplemental training courses in the use of specific modelling software (TOUGH2 and ANSYS), as well as from fellowships, which allowed some of the participants to obtain additional knowledge and experience in the use of numerical simulation tools;

- While the flow and transport simulators used as part of this CRP did not present a technical challenge to the participants, it must be noted that only basic processes were considered. Some participants explored the use of more sophisticated simulators that can handle coupled hydrological, thermal, and mechanical processes. However, coupled biogeochemical and geophysical processes were not considered, neither was inverse modelling. Obtaining experience in advanced simulation capabilities is highly technical and best achieved through short courses and extended fellowships;
- Despite the fact that all participants came from non-English speaking countries, communication during the RCMs was very good. However, there appears to be a need to substantially improve the quality of written documents, specifically on the presentation of concepts, scientific results, analyses, and conclusions. Providing training in structuring and writing technical documents may be beneficial to the international community involved in nuclear waste isolation projects;
- This CRP was aimed at transferring knowledge and expertise to the appropriate research institutions in the Member States. For this transfer to be successful, it is essential that the CRP activities are aligned with the Member State's interests, and that the expertise gained by the individuals participating in the CRP is disseminated among the technical staff at their home institutions. Continuing education in numerical modelling is required within and outside of IAEA-sponsored networks to ensure a successful transfer of simulation technology;
- Most of the participants expressed their opinion that the CRP was useful and helped them advance their understanding of modelling approaches in support of their nuclear waste isolation programmes. Whether this CRP achieved its stated goals of transferring modelling expertise may be further examined by soliciting specific feedback from the participants. Future CRPs are likely to benefit from such an evaluation;
- An early kick-off meeting would have helped guide and streamline the simulation studies, making the CRP more effective.

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Annex I

DESCRIPTION OF SEMI-GENERIC SITE

The purpose of the description of the Veresnia site is to present the data about one of the Ukrainian sites potentially suitable for geological disposal of radioactive waste. The presented data were used by all participants of the IAEA's Project CRP T2.10.24 as the common basis for far field conceptual and numerical modelling. A comparison of the Veresnia site to two Scandinavian sites is also presented.

I-1. GENERAL DESCRIPTION

I-1.1. Location

The Veresnia site (Fig. I-1) is located in the northern part of the Ukraine in the watershed area of the Uzh (tributary of Prypiat) and the Teteriv (tributary of Dnieper) rivers. The site covers an area of 290 km^2, forming a square with a side length of 17 km. The Veresnia site belongs to the Polessie administrative district of the Kyiv region. In the north-east, the Veresina site borders the Chernobyl Exclusion Zone (CEZ). The approximate distances from the site borders to some characteristic locations are:

- To the City of Kiev (population 2 800 000): 75 km;
- To Chernobyl NPP: 30 km;
- To the town of Korosten (population 67 000): 60 km;
- To Belarus Republic state border: 25 km.

FIG. I-1. Location of Veresnia site (green line: site borders; red line: CEZ borders, blue line: area of regional geological map shown on FIG. I-2).

I-1.2. Climate

The Veresnia site is located in a zone of moderate-continental climate with a positive moisture balance. The average annual precipitation (600 mm/year) exceeds the evaporation potential. The maximum daily precipitation is in July (76 mm), and the minimum in March (37 mm). The average annual evaporation is 524 mm with monthly maximum in July (98 mm), and minimum in December (1 mm).

The climatic conditions of the site are influenced by marine and continental air masses. In the summer and autumn, westerly and north-westerly winds prevail, whereas south-easterly winds prevail during the cold period.

The average annual air temperature is +6.7^{o}C. The warmest month is July (average temperature +19^{o}C); the coldest month is January (-6^{o} C). A stable snow cover exists from mid-December to mid-March, with an average thickness of 0.17 m.

I-1.3. Relief and landscape

The site is located within the Polessie Lowland in the north-eastern part of the Kiev moraine sandur plain. Characteristic for the area is its hilly-plain topography with comparatively low elevation differences (less than 20 m). The absolute elevation decreases from 165-175 m in the south-western part of the site to 130-140 m in the northern and eastern parts. The highest elevation is 198 m. The absolute elevation of river banks varies from 125 to 130 m.

The site is characterized by general accumulative relief represented by two formation types:

- Relief formed as a result of fluvioglacial accumulation – moraine sandur plain;
- Accretion-denudation relief formed by water courses and aeolian processes.

According to Ref. [1], the major landscape types over the studied area are associated with the depressed, slightly hilly moraine-glacial plain on the Paleogene-Neogene basement overlain by boulder loams and sands of variable thickness. Typical for the area are sod-podzol soils mostly covered by coniferous and mixed (coniferous-deciduous) forests, and occasional tilled land.

I-1.4. Hydrology

The largest rivers in the region are the Prypiat and Teteriv (right tributaries of the Dnieper), and the Uzh (right tributary of the Prypiat). The basic hydrological characteristics of these rivers are given in Table I-1.

TABLE I-1. HYDROLOGICAL CHARACTERISTICS OF THE RIVERS PRYPIAT, TETERIV AND UZH [1]

River	Minimum distance to boundaries of Veresnia site (km)	River length (km)	Drainage area (km^2)	Average annual flow runoff modulus, at the river mouth ($l/s \cdot km^2$)	Annual runoff volume (km^3) with probability (%)	
					50%	95%
Prypiat	30	761	114 300	3.7	13.2	6.82
Teteriv	15	365	15 300	2.7	0.74	0.35
Uzh	6	256	-	-	0.47	-

There are also small rivers passing through the Veresnia site: the Bober and Radinka (tributaries to the Uzh river), and the Veresnia and Oleshnia (tributaries to the Teteriv). They have a width of less than 10-15 m, a depth of about 1.5-2 m, flow velocities of 0.1-0.2 m/s, and flow rates of approximately 1.5-3 m^3/s. The river valleys are swamped in some places.

I-1.5. Population, economic activity, groundwater use

Prior to the Chernobyl accident, the population of the Polessie administrative district (area 1300 km^2) reached 30 000, with a density of about 23 persons/km^2. More than half of the inhabitants lived in the countryside. The land types were distributed by area as follows: croplands 35%; forests and bushes 53%; bogs, rivers and lakes 3.3%; meadows 2.2%; gardens 0.2%; roads 0.1%; rural development 4.8%; and urban development 1.7%.

Characteristic for agricultural crops are flax, hop, potato, winter wheat, rye, barley, and oats. Cattle-breeding is poorly developed. The mining industry in the Polessie administrative district is represented by building materials recovery (sand, clay), and peat recovery.

After radioactive contamination of a part of the territory caused by the Chernobyl accident, a number of inhabitants resettled in clean areas. At present, up to 4000 people live within the Veresnia site, with an average population density of 13 persons/km^2 [2].

The population uses the groundwater of the Quaternary aquifer for drinking and domestic needs, and of the Eocene aquifer as water supply for the cattle farms (see also Section I.2.6). The water supply is decentralized and realized mainly by water extraction from individual shallow wells. The total groundwater production used for water supply in the Veresnia site is 50-60 m^3/day.

I-2. GEOLOGICAL DESCRIPTION

I-2.1. Regional setting

Most of the available information about the crystalline basement structure (see Fig. I-2) within the study area has been obtained from geophysical, geomorphological and neotectonic investigations presented in Refs [3-5].

Three major geological structures are distinguished, stretching from SW to NE. They are (1) the Korosten Pluton, (2) the east fringe of the Korosten Pluton, and (3) the Dnieper-Donetsk

Depression (DDD). The crystalline basement of the study area is dissected by three large faults: (1) the Pre-Cambrian Teteriv Fault with NE strike, (2) the Prypiat Fault of latitudinal strike, and (3) the Phanerozoic Kyiv Fault of NW strike parallel to the SW slope of the DDD.

The western part of study area is occupied by the Korosten Pluton. It has almost isometric form, is up to 150 km wide in the WE direction and 110 km wide in the NS direction, covering a total area of about 12,000 km^2. Most of the Korosten Pluton is composed of rapakivi and rapakivi-like granites, underlying and overlaying the bedded anorthosite bodies. The intrusion is of 3-6 km thick. The Korosten Pluton is bounded by a circular system of normal faults. The intensively dislocated Early Proterozoic metamorphic rocks (of the Teterev and, probably, Bug series) are penetrated by granitoids of the Zhytomir complex and serve as enclosing strata for the Korosten Pluton formations.

Most of study area, including the Chernobyl NPP operation site, is situated within the east fringe area of the Korosten Pluton (between the Pluton and DDD) with a width of 40-60 km. The fringe area is extended in NW direction parallel to the contact line with the Pluton. The geological composition of the territory is extremely complicated. Evidently, the crystalline basement is composed of paleogranite, gneiss or granodiorite with subordinated bodies of basic rocks (probably, ultra-basite) of Archean and Early Proterozoic ages. These rocks are substantially metamorphized and elastically deformed. In the crystalline complex composition the plagiogranites dominate (70-80%) within the Pluton fringe area, whereas the basic rocks form relatively large isolated bodies (3-5 km in diameter). Zones of concentration of basic rock bodies are present comprising about half of the crystalline massif. These zones are associated with the exocontact zone of the Korosten Pluton, having a width of 4-5 km, and sometimes up to 10 km (in the north-eastern part of the Veresnia site), and the area located NW of the Chernobyl NPP.

The granitoids occurring within the Korosten Pluton fringe area are more dense and magnetized than the Korosten granites, and they are similar to the metamorphized Archean plagiogranites of the Bila Tserkva, Kryvyi Rig and Middle Dnieper regions. Analogously, basic rocks of the fringe area are similar to the greenstone formations. The contact between basic and acid rocks is dipping mainly at a steep angle. Acid rocks (paleogranite and gneiss) are composed of plagioclase, quartz and biotite, with lower abundance of hornblende. The basic rocks are represented by amphibolite and are composed of plagioclase and hornblende, in rare cases containing biotite. The rare occurrence of ultrabasites consists of actinolite or chlorite-talc-carbonate rocks.

TABLE I-2. SOME ROCK PROPERTIES AT THE VERESNIA SITE

Depth interval (m)	Description	Geological index	Specific density (g/cm^3)	Porosity (%)
0-250	Sediments: sands, chalk, marls, aleurite, argillite	MZ-KZ	$\frac{1.71\ldots2.31}{2.0}$	Up to 20
250-500	Korosten complex: biotite-hornblende rapakivi-like granites, of middle-ovoid and large-ovoid structure	$\gamma r^1 PR_2 ks$	$\frac{2.55\ldots2.67}{2.61}$	Up to 1
500-1100	Korosten complex: biotite-amphybolite rapakivi-like granites of no-ovoid and small-ovoid structure	$\gamma r^2 PR_2 ks$	$\frac{2.58\ldots2.66}{2.62}$	0.2…0.6
1100-4000	Korosten complex: amphybolite-biotite rapakivi-like granites with olivine and pyroxene	$\gamma r^3 PR_2 ks$	$\frac{2.61\ldots2.69}{2.65}$	0.2…0.4

Geologically, the Veresnia site is situated at the NE margin of the complex-structured Korosten Pluton. The ultra-metamorphic and intrusion formations of the crystalline base with terrigenous and carbonate formations of sedimentary cover compose the geological structure of the site (see Table I-2). The depth of crystalline basement occurrence changes from 150 m in the western to 250 m in the eastern part of the site, so that the upper rigidity frame boundary gradually deepens to the east, with increasing thickness of sedimentary rocks.

I-2.2. Sedimentary cover

Within the site area the sedimentary formations contain a discontinuous weathering crust with a thickness of 0 to 58 m, consisting of remains of Paleozoic-Mesozoic age. The weathering crust is overlaid by Middle Jurassic sandy-clay and marl formations with a thickness of up to 95 m. As a stratigraphic anomaly, the Upper Cretaceous sandstone-limestone deposits occur with thickness to 20 m occur over the Middle Jurassic formations, and are covered by Paleogene-Neogene aleurites, marls, sands, clays and silica of total thickness about 60 m. The sedimentary section is completed by sandy-clayey, mostly glacial formations with a thickness to 50 m.

All beds are composed of permeable rocks (sands, sandstones, fractured chalks, etc.), forming aquifers of local and regional scale. Clays, marls and aleurites serve as confining beds. Within river valleys, where sedimentary deposits are washed out, the aquifers may joint each other, forming an interrelated aquifer system.

I-2.3. Crystalline rocks

Rocks of crystalline basement are represented by ultra-metamorphic early Proterozoic formations of Zhytomir complex and intrusive Middle Proterozoic formations of Osnitsa and Korosten complexes (see Fig. I-2). The description of these rocks follows that given in Ref. [6].

Zhytomir complex: The granite massifs of the Zhytomir complex vary by area from 20 to 300 km^2. They occur west, south and east of the Korosten Pluton. Typical zhytomir granite is light grey, is uniform medium-grained and has a bulk or gneiss-like texture. Its mineral composition includes plagioclase 34.7%, potash feldspar 28.7%, quartz 25.1%, biotite 7.7%, and muscovite 3.2. The associated minerals are represented by monazite, zircon, apatite, sulfides, molybdenite, ilmenite, and magnetite. Zhytomir granites are of uranium-phosphorus geochemical type. The age of the granites is 2020-2080 Ma.

Ostnitsa complex: The massifs of the Osnitsa complex occur as a sub latitudinal band north from the Korosten Pluton. These massifs are composed of coarse-grain and fine-grain leucocratic and melanocratic granites, granodiorites, and diorites. The Osnitsa granites vary from pink to red. They are porphyry-like or uniform-grained, bulk, coarse- and medium-grained, with characteristic lilac-colored quartz. They are typically composed of microcline 30-46%, plagioclase 14-28%, quartz 21-49%, biotite 1-11%. The composition of granodiorites includes also hornblende. The accessory minerals are represented by zircon, apatite, sphene, magnetite, ilmenite, garnet, corundum, tourmaline, rutile, orthite, and fluorite. The age of these rocks is 1980-2010 Ma.

Korosten complex: The Korosten complex consists of hornblende-biotite rapakivi-like granites of small-ovoid structure. They are represented mostly by reddish-brown, greyish-red or greenish-grey (at greater depth) porphyraceous rocks with fine-, medium- and coarse-grained body. The mineral content is as follows: potash feldspar 50-60%; quartz 25-30%; plagioclase 10-25%; biotite 0.5-5%; hornblende 0.5-4%; pyroxene and olivine up to 1%.

Within the Korosten Pluton, large-ovoid hornblende-biotite rapakivi granites are less frequent. They represent greenish-grey and foxy massive rocks composed of large (up to 2-5 cm) ovoid microcline with oligoclase fringe included into a medium-grained body. The latter is composed of potash feldspar, plagioclase, quartz and biotite. Small proportions (up to 1-2%) of monoclinic pyroxene and olivine can be found almost everywhere together with secondary minerals: chlorite, carbonate, serpentine, prehnite, sericite, and accessory minerals: magnetite, ilmenite, fluorite, zircon, apatite, orthite, tourmaline, and sphene.

In the north-western part of the Korosten Pluton, the biotite granite-porphyry is abundant as pink, brownish-pink, occasionally black fine-grain rocks of porphyric structure. Granite-porphyry forms numerous dikes and stock-like bodies.

The age of the Korosten complex is estimated as ranging from 1660 to 1640 Ma (by biotite using potassium-argon method), and from 1760 to 1600 Ma (by zircon in rapakivi-granite using uranium-thorium-leaden method).

I-2.4. Tectonics and neotectonics

The major tectonic dislocations within the Veresnia site are (1) the Teteriv Fault zone of NE direction, which is of deep mantle origin (according to data from deep seismic soundings); and (2) the regional Kyiv Fault of crustal origin.

The Teteriv Fault zone is sub vertical, sometimes steeply sloping. It is of fault type, and its elevated north-western block forms a horst structure, and the south-eastern block deepens by its stairs in south-eastern direction. Outside of the site (in north-eastern direction) in places where the Teteriv Fault crosses the Dnieper-Prypiat Depression, the Teteriv zone involves rocks of the traprock formation of Devonian age, which indicates its intensive activation in the Hercynian foldering epoch. Additional studies of seismic safety for Rivne and

Khmelnitsky NPPs have discovered neotectonic activity of the Teteriv Fault zone at many of its sections, SW from the Veresnia site.

The Kyiv Fault is of NW direction. It deepens in south-western direction at angles from 90° to 45°. The available information is not sufficient to decide about its possible activation in more recent epochs.

According to geophysical data, all other breaks are of secondary order, though some of them extend beyond the studied area. Most of them are of diagonal and sub-latitudinal directions and belong to block-internal type.

Neotectonic parameters involve amplitude of Late Oligocene-Anthropogen (app. 25 Ma) and Holocene-Pleistocene (app. the last 1 Ma) movements.

Typical for the Veresnia site are positive amplitudes of the neotectonic movement. Maximum amplitude of Neogene uplift of the Earth crust was revealed within the Korosten Pluton (170-200 m), the minimum one is in the fringe area (near Chernobyl – 110 m). The maximum amplitude of Holocene-Pleistocene crustal uplift also occurs within the Korosten Pluton (20-40 m) and much less (up to 10-20m) within the fringe area. Individual sites with high gradients of neotectonic movement velocity (0.5-3 mm/km per thousand years) have been identified.

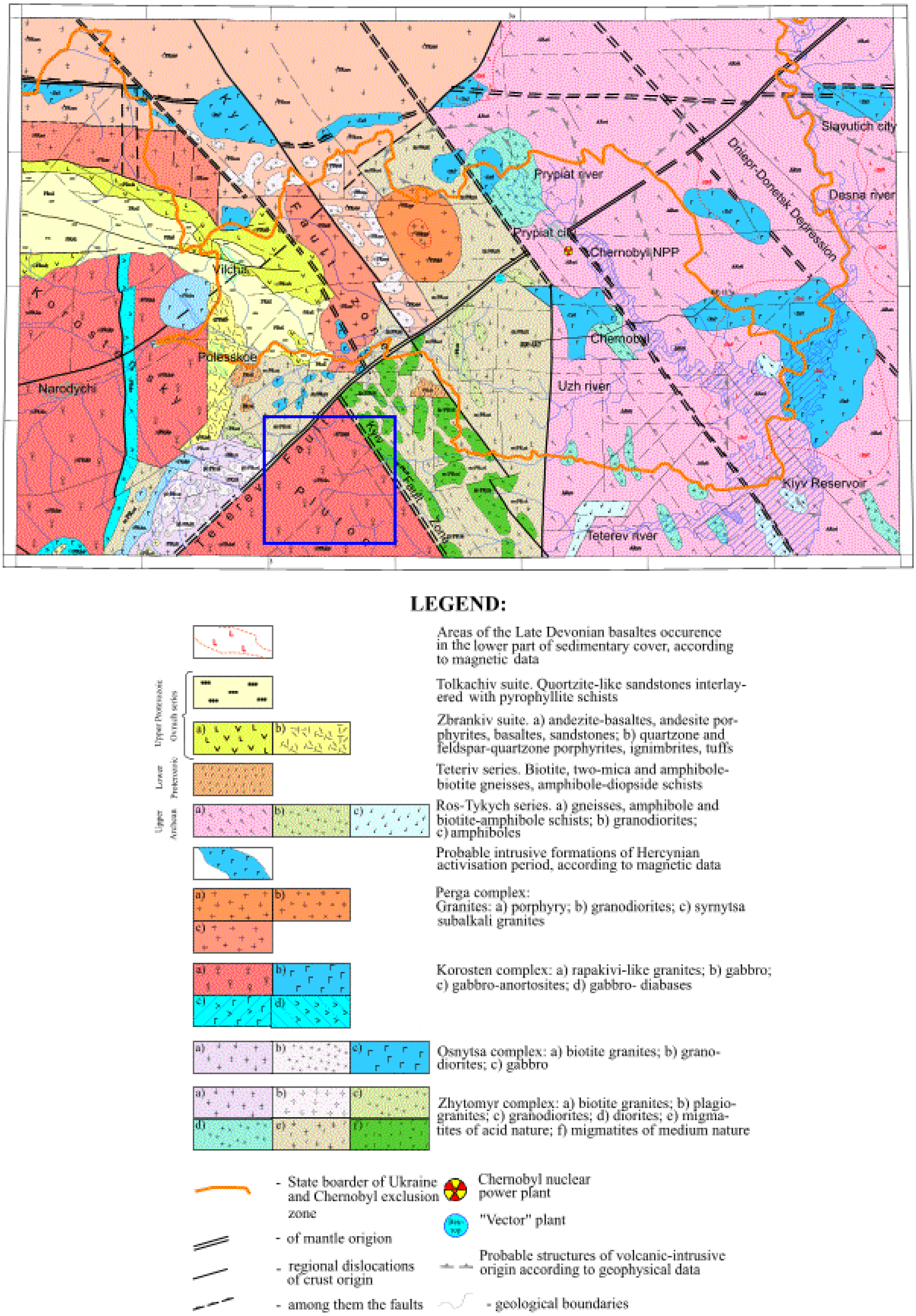

FIG. I-1. Regional geological map of crystalline basement of CEZ and its neighbourhoods (according to Refs. [4, 5]).

I-2.5. Fracturing

Data about the fracturing of crystalline rocks of the Veresnia site have been obtained by drilling of a special borehole located near the village of Budynychi, which is located northwest of the site and exhibits analogous geological conditions.

The borehole discovered biotite-amphibolite, no-ovoid and small-ovoid rapakivi-like granites of the Korosten complex ($\gamma r^2 PR2ks$) to depths of about 500 m. As is seen from the section, the upper part of crystalline rocks to a depth of 370 m has rather high specific fracturing (10-15 fractures per meter of borehole), gradually decreasing with depth. The nature of this fracturing is related to exogenic processes, which decrease with depth. Below the depth of 350 m, the fracturing is significantly lower, and only locally endogenic fractures appear related to internal-block tectonic breaks.

The thickness of vein formations in granites is usually low, on the order of 0.1 mm, occasionally reaching 1-2 mm. The surface area of open fractures varies from 1-4 mm^2 (in dense rocks), and up to 15-20 mm^2 (in high fractured zones) per 1 m of the core sample. The volume of vein formations does not exceed 2-5 % of the granite massif volume. The minerals of vein formations in the upper granites section (first 20-30 m) are represented by limonite, goethite, haematite, siderite, and tiff. In deeper horizons (500-600 m) the vein fractures contain hydromica, chlorite, kaolinite, quartz, anatase, and baryte.

I-2.6. Hydrogeology

Three aquifers exist in the sedimentary cover of the Veresnia site:

- Quaternary;
- Eocene;
- Cenomanian-Callovian.

Four hydrodynamic zones are distinguished in the crystalline basement:

- Zone of intensive water exchange (a few hundred meters of thickness);
- Zone of significant water exchange (to a depth of 1000 m);
- Zone of retarded water exchange (depth range of 1000 – 2500 m);
- Zone of extremely retarded water exchange (the depth under 2500 m).

The basic uncertainties are associated with the fact that within the study area the hydrogeological characteristics are available only for aquifers of the sedimentary cover and the weathering zone of the crystalline rocks. The information about deep horizons is of hypothetical character.

Quaternary aquifer: Hydraulic conductivity varies between $6 \cdot 10^{-6}$ and $2 \cdot 10^{-4}$ m/s. The average transmissivity is $6 \cdot 10^{-3}$ m^2/s for the deposits in the riverside zones of the local hydrographical system, and $6 \cdot 10^{-4}$ m^2/s over the rest of the territory. The amplitude of the annual groundwater table fluctuation is 0.3-1.5 m. The main source of groundwater recharge for the Quaternary aquifer system is atmospheric precipitation.

The groundwater chemical composition is hydro carbonate calcium, sodium chloride. The mineralization varies from 0.1 to 1 g/l. The water is used by local residents of the Veresnia site for home purposes and drinking water supply.

Eocene aquifer: This aquifer is separated from the quaternary aquifer by a low-permeable, 10-20 m thick layer of the Kiev suite marls. The aquifer is artesian. Small hydraulic "windows" in the confining bed have been observed. They facilitate vertical water exchange between the Neogene-Quaternary and Eocene aquifer systems. Hydraulic conductivity of the Eocene sands varies from $6 \cdot 10^{-6}$ to $3 \cdot 10^{-4}$ m/s. The average transmissivity for the Eocene water-bearing deposits is $5 \cdot 10^{-3}$ m^2/s in the riverside zones of the local hydrographical system, and $8 \cdot 10^{-4}$ m^2/s over the rest of the territory. The Eocene water-bearing sands overlie the Upper Cretaceous marl-chalk layer. The latter serves as a regional aquitard, separating the confined Eocene and Cenomanian-Callovian aquifer systems. The hydraulic conductivity of the relatively low-permeable Kiev marls I son the order of 10^{-7} m/s.

The chemical composition of the groundwater is hydrocarbonate calcium, less frequently sulfate calcium-magnesium. The mineralization reaches 1 g/l. The water is used for water supply of farms within the Veresnia site, and for drinking water supply for the city of Chernobyl and the Chernobyl NPP.

Cenomanian-Callovian aquifer: The hydraulic conductivity of these deposits ranges from $5 \cdot 10^{-6}$ to $2 \cdot 10^{-4}$ m/s. The Cenomanian-Callovian aquifer system is underlain by Bathonian-Callovian low-permeable layer of clays and aleurites, with frequently occurring hydraulic "windows". This layer serves as a confining bed between the upper Cenomanian-Callovian and the lower Bajocian (Middle Jurassic) aquifer systems. The hydraulic conductivity of the Upper Cretaceous compact marls is on the order of 10^{-8} m/s.

The chemical composition of the groundwater is hydrocarbonate calcium, hydrocarbonate magnesium-sodium-calcium, chloride-hydrocarbonate sodium with mineralization to 0.7 g/l. The groundwater is intensively used for water supply of the city of Kiev.

The groundwater in the highly fractured upper zone of the crystalline rocks *(zones of intensive and significant water exchange*) forms a single aquifer. This aquifer is confined (pressure head is 0-40 m, averages 10-30 m). Hydraulic conductivity ranges from $3 \cdot 10^{-6}$ to $2 \cdot 10^{-5}$ m/s for fractured crystalline rocks in the zone of active water exchange. The average hydraulic conductivity is $1 \cdot 10^{-6}$ m/s in the riverside zones, and $1 \cdot 10^{-7}$ m/s in the rest of the territory. The hydraulic conductivity of the confining bed in the roof of the crystalline basement shows the noticeable upward trend in W-E direction from $6 \cdot 10^{-8}$ to 10^{-8} m/s.

Occurrence of highly mineralised groundwater may serve as an indication of the *zone of retarded* and *zone of extremely retarded water exchange*. Within the Korosten Pluton borders, a zone of mineralised water has not been identified. According to preliminary assessments at a depth of 1500 m, the hydraulic conductivity of massive crystalline rocks ranges from $2 \cdot 10^{-7}$ to $2 \cdot 10^{-8}$ m/s; at a depth of 2500 m, it ranges from $1 \cdot 10^{-7}$ to $1 \cdot 10^{-8}$ m/s [5]. Hence, within the Korosten Pluton the groundwater flow rate in the zone of retarded water exchange of the basement must be three orders of magnitude less than in the zone of active water exchange.

I-3. COMPARISON TO SKANDINAVIAN SITES

I-3.1. Hydrological properties of Finnish bedrock

Table I-3 shows the hydraulic conductivity (K) of intact crystalline rocks and hydraulically conductive fractures at the Olkiluoto site [7]. The main rock type of this site is migmatitic mica gneiss. Less frequent rock types include granites, tonalities, quartz feldspar gneisses and amphibolites. The frequency of hydraulically conductive fractures varies from 0.1 to 0.3 per meter. The conductive fractures are mainly defined as filled (70 to 80% of all fractures). Typical infillings are carbonates, sulphides, clay minerals and chlorites.

TABLE I-3. HYDRAULIC CONDUCTIVITY K (M/S) OF THE INTACT ROCK AND HYDRAULICALLY CONDUCTIVE FRACTURES AT THE OLKILUOTO SITE

Rock type	lg K in m/s (2 m scale)			
	Arithmetic mean	Standard deviation	Range of variation	Count
Migmatitic mica gneiss				
Intact	-8.3	0.8	-9.7 to -6.2	140
Fractures or crushed zones	-6.4	1.6	-9.0 to -5.0	42
Granites				
Intact	-7.9	0.8	-9.3 to -6.3	65
Fractures or crushed zones	-6.1	0.8	-8.3 to -5.0	31

I-3.2. Hydrological properties of Swedish bedrock

Data about K-values for three Swedish sites are given in Tables I-4 and I-5 [8].

TABLE I-4. SUMMARY OF HYDRAULIC CONDUCTIVITY VALUES (25 M SCALE) FOR THREE SWEDISH SITES

Parameter	Aberg (granite, greenstone)	Beberg (diorite, granodiorite)	Ceberg (sedimentary gneiss)
Mean of lg K for rock mass (m/s)	–8.8 to –7.1	–7.2 to –6.4	–10.3 to –8.9
Mean of lg K for fracture zones (m/s)	–8.3 to –5.3	–7.5 to –4.3	–9.6 to –6.9
Standard deviation of lg K for rock mass and fracture zones	1.6	0.8	1.1

TABLE I-5. VERTICAL ZONALITY OF K-VALUE (m/s) FOR BEBERG AND CEBERG SITES ON 25 M SCALE

Depth interval (m)	Beberg Arithmetic mean lg K	Depth interval (m)	Ceberg Arithmetic mean lg K
		+110 to 0	–7.6
above –100	–6.6 to –6.8	0 to –100	–9.0
–100 to –200	–7.2 to –7.8	–100 to –300	–10.0
–200 to –400	–7.8 to –8.1	below –300	–10.3

I-4. CONCLUSIONS

The geological and surface characteristics of the Veresnia site are very similar to Scandinavian sites (Forsmark, Olkiluoto) regarding age, material composition (petrographic, mineralogical), degree of tectonic transformation, groundwater permeability properties of crystalline rocks, and the ecosystem characteristics.

The differences between the Veresnia and Scandinavian sites are:

- Climatic characteristics (the Veresnia site is located in warmer climatic conditions with higher evaporation. This results in lower groundwater infiltration recharge);
- Presence in the Veresnia site of developed sedimentary cover with several water-bearing horizons;
- Groundwater sources and formation history (Veresnia is continental, whereas the Swedish and Finnish sites are close to the sea, leading to differences insalinity and chemical composition).

References to Annex I

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[2] MINISTRY OF EMERGENCY OF UKRAINE, CD Atlas of Radioactive Contamination of Ukraine, Ministry of Emergency of Ukraine, Kiev (2002).

[3] SHESTOPALOV, V., et al., Geological Disposal of Radioactive Waste in Ukraine (Problems and Solutions) (SHESTOPALOV, V. Ed.), NAS of Ukraine, REC, Kiev (2006).

[4] SCIENTIFIC AND TECHNOLOGICAL CENTRE OF UKRAINE, Scientific and Technical Grounds for ChNPP Radioactive Wastes Disposal in Deep Boreholes Completed in Korosten Crystalline Massif., Project 1396, Final Report, STCU, Kiev (2003).

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[8] SKB, Deep Repository for Spent Nuclear Fuel, SR 97 – Post-Closure Safety, Report TR 99-06, SKB, Stockholm, Sweden (1999).

Annex II

COUNTRY SPECIFICATIONS

CHINA	
Waste type	RBMK-1500 SNF
Amount	2.04 tU per canister
Cooling time	40 years
Ref. RN inventory	See Ref. [1], p. 14, Table 3-3.
Selected RNs NF	Ag108m, Am241, Am243, C14, Cl36, Cm245, Cs135, Cs137, Ho166m, I129, Nb94, Ni59, Ni63, Np237, Pa231, Pd107, Pu239, Pu240, Pu242, Ra226, Se79, Sm151, Sn126, Sr90, Tc99, Th229, Th230, U233, U234, U235, U238, Zr93.
Selected RNs FF	I-129 and Se-79
Container type	Copper canister, 50 mm thick
Container release function (for NF model)	The canister defect growing time (initial 1 mm^2 hole, growing stepwise to 0.01 m^2) and the time of groundwater contact with SNF were assumed to be constant (200 000 years)
Matrix leaching rate	Deterministic analysis: 10^{-7} $year^{-1}$ based on SKB report
IRF	Ref. [1], P.17, Table 3-4.
Disposal concept	KBS-3 concept
Repository layout	KBS-3 concept
Reference site	semi-generic UKR site
FF model type	Simplified semi-generic UKR site, summary was provided in CPR report 2009.
RN migration parameters	Ref. [1]
References	[1] LINDGREN, M., LINDSTRÖM, F., Radionuclide transport calculations, Report TR-99-23, SKB, Stockholm (1999).

LITHUANIA	
Waste type	RBMK-1500 SNF
Amount	2440 tU
Cooling time	50 years
Ref. RN inventory	The radionuclide transport analysis was performed for the RBMK-1500 SNF with initial enrichment of 2.8 % ^{235}U and 0.6 % Er_2O_3. The SNF burnup is approximately 29 MWd/kgU, the radionuclide inventory was assessed by SAS2H (computer code system SCALE 5). Data on possible impurities in the fuel itself and its structural parts have been taken into account based on literature sources.
Selected RNs NF	Deterministic analysis: Safety relevant radionuclides identified for RBMK-1500 SNF as reported in Ref [1]. Probabilistic analysis: the radionuclides with more significant release from the Near field as it had been observed in the deterministic analysis: Ni-59, Se-79, Nb-94, I-129, Cs-135, Ra-226 and its predecessors from decay chain (Pu-242, U-238, U-234, Th-230)
Selected RNs FF	I-129 as it was decided at RCM3, LEI, Kaunas, Lithuania, 9-13 Nov., 2009
Container type	Copper canister, 50 mm thick
Container release function (for NF model)	Deterministic analysis: Reference scenario: the canister defect growing time (initial 1 mm^2 hole, growing stepwise to 0.01 m^2) and the time of groundwater contact with SNF were assumed to be constant (200 000 years) based on Ref. [2]. Probabilistic analysis: • Scenario A (canister defect scenario): the canister defect growing time and the time of groundwater contact with SNF were assumed to be constant (200,000 years) based on Ref. [2]. Defect size is the same as in deterministic analysis. • Scenario B (the canister defect scenario): canister defect could become larger at any time between 1000 and 100 000 years (triangular distribution) after repository closure and continuous groundwater pathway forms after 1000 years based on Ref. [3]. Defect radius before enlargement is r=2 mm; after enlargement r=1000 mm based on [3]. • Scenario C (climate change scenario): canister defect growing time and the time of groundwater contact with SNF were assumed to be constant (100 000 years), based on assumption on repetition of the last glacial/interglacial period in Lithuania.
Matrix leaching rate	Deterministic analysis: 10^{-7} $year^{-1}$ based on SKB report [4]. Probabilistic analysis: Triangular probability distribution function based on SKB report [4] and summarized in Table 5 in LEI draft country report [5]

IRF	<u>Deterministic analysis:</u> Medium values based on SKB report [4] which are summarized in Table 4 in LEI report [6]. <u>Probabilistic analysis:</u> Triangular probability distribution functions based on SKB report [4]and summarized in Table 5 in LEI draft country report [5].
Disposal concept	For the deterministic analysis, the KBS-3V concept was assumed. A short summary is provided in LEI report [6]. For the probabilistic analysis, the KBS-3H concept was accepted. A short summary was provided in LEI draft country report [5].
Repository layout	
Reference site and far field model type	The reference site is consistent with the semi-generic site Veresnia (UKR) site, as described in UKR report [7] and Annex I. The model geometry, hydraulic properties, and boundary conditions are as defined in LEI draft country report [5].
Radionuclide migration parameters	One defect canister. Parameter values for the assessment of radionuclide transport in the near field as defined in LEI draft country report [5] and in the table above.
Additional scenario details	Continuous porous medium approach is assumed for far field modelling. Different cases with and without regional flow and with three different well drawdown have been evaluated. Various canister defect and climate change scenarios were analysed.
References	[1] BRAZAUSKAITE, A., POSKAS, P, Radionuclide migration from the geological repository of the RBMK-1500 Spent Nuclear Fuel in Crystalline Rocks. 2. The identification of safety relevant radionuclides, Power Engineering. Vol. 2. 2006. P. 47-56 (In Lithuanian). [2] SR 97 – Post-closure safety. SKB Technical Report TR-99-06, 1999. [3] Long-term safety for KBS-3 repositories at Forsmark and Laxemar – a first evaluation. Main Report of the SR-Can project, SKB Technical report TR-06-09, 2006, 620 p. [4] Spent fuel performance under repository conditions: A model for use in SR-Can, SKB Technical Report TR-04-19, 2004, 34 p. [5] Justinavičius, D., Narkūnienė, A., Poškas, P., Poškas, R. The Use of Numerical Models in Support of Site Characterization and Performance Assessment Studies of Possible Geological Repository in Clay Formation in Lithuania. Draft Country Report, February 2010. [6] Brazauskaitė, A., Poškas, P., Poškas, R. The Use of Numerical Models in Support of Site Characterization and Performance Assessment Studies of Possible Geological Repository in Clay Formation in Lithuania, Progress Report, August 29, 2007. [7] Shybetskyy, S., Shestopalov, V., Boguslavskyy, and B. Stetsenko. Description of Veresnia Site (Ukraine) and some Hydrogeological Properties of Crystalline Rocks, Data Report, December 12, 2006.

ROMANIA	
Waste type	CANDU-6 SPENT FUEL irradiated to an average burnup of 685 GJ/Kg U (7928 MWd/tU) and cooled for 40 years after discharge from a CANDU 6 reactor
Amount	Spent fuel resulted from four nuclear CANDU units: 812,160 fuel bundles, 15,396.93 t U [1].
Cooling time	10 Years (conservative approach); 40 Years (realistic approach) for TH modelling [2]
Ref. RN inventory	ORIGEN-S radionuclide generation and depletion code has been used to predict RN inventory in the fuel and zircaloy cladding and of radionuclide produced by neutron activation of impurity in both UO_2 fuel and Zircaloy cladding [2]
Selected RNs NF	I-129, Se-79
Selected RNs FF	I-129, Se-79
Container type	The disposal container is a packed-particulate used-fuel disposal container fabricated from ASME Grade-2 titanium, which holds 72 used fuel bundles [3].
Container release function	Catastrophic failure after 500 years (conservative approach [3])
Matrix leaching rate	9.0×10^{-5} year^{-1} (best estimate value) and 2.6×10^{-9} year^{-1} (sensitivity analysis) [3]
Instant release fractions	0.1% of Ni, Mo, Nb; 0.8% of actinides; 1% of Sm; 2% of Pd, Sn; 3% of C, Sr, Zr; 5% of Cl, Rb; 6% of Tc; 8% of Se, I, Cs [3]
Disposal concept	Ref. [3]
Repository layout	Ref. [3]
Reference site	Veresnia (Ukraine) [4]
Far field model type	Ref. [2, 3]
RN migration parameters	Refs [2, 3]
Additional scenarios	-

References	[1] JOHNSON, L.H., et al., The Disposal of Canada's Nuclear Fuel Waste: The Vault Model for Postclosure Assessment, AECL-10714, COG-93-4, 1994. [2] ILIE, P., et al., The Development of Numerical Models and Computer Codes in Support of Siting and Performance Assessment Studies of Geologic Repository in Crystalline and Igneous Rocks, Contract Report, 2008. [3] ILIE, P., et al., Groundwater Flow and Near-Field Source Term and Thermal Analysis, Progress Report, September 4, 2007. [4] SHYBETSKYY, Y., et al., Description of Veresnia Site (Ukraine) and some Hydrogeological Properties of Crystalline Rocks, Data Report, December 12, 2006.

UKRAINE[2]	
Waste type[3]	RBMK-1500 SNF with a burnup 29 MWd/kg [1]
Amount[4]	1.77 tU (calculated on base of Ref. [1])
Cooling time [5]	50 years, as it defined in Ref. [1]
Ref. RN inventory[6]	See Reference [8] from Ref. [1]
Selected RNs NF	RN's release in the near field was not simulated (data from Ref. [2] were used)
Selected RNs FF	^{129}I , ^{79}Se – for transport modelling; Sr, Cs, Tc, U, Np and Pu – for preliminary studying of sorption
Container type[7]	Swedish type copper container [1]
Container release function	As it is defined in Ref. [2] for one defected canister scenario: release starts at 200 000 years after container emplacement
Matrix leaching rate	10^{-7} $year^{-1}$ [1]
Instant release fractions	Values with maximum probability from Ref. [3]
Disposal concept & Repository layout8	KBS-3V concept, as it is described in Ref. [1]
Reference site	VERESNIA site (Ukraine), as it is described in Ref. [4].
Far field model type	Continuous porous medium without and with a fault zone as it is shown in Ref. [4] Model geometry, hydraulic properties & boundary conditions as in Ref. [4]

2 The table contains generalized information on suppositions and parameters used by the UKR team to model groundwater flow and radionuclide transport in the framework of UKR13374 Project implementation. These data do not always correspond to characteristics of Ukrainian SNF.

3 BWR SNF from RBMK-1000 reactors and vitrified HLW after processing of PWR SNF from WWER-440 and WWER-1000 reactors

4 For Ukraine: appr. 110 m^3 of vitrified HLW after processing of WWER-440 reactors; appr. 1230m^3 of vitrified HLW after processing of WWER-1000 reactors; 2400 tU – SNF from RBMK-1000 reactors.
SNF from WWER-440 and WWER-1000 (partially) reactors of Ukrainian NPPs is transported for reprocessing to Russian Federation. Reprocessing of WWER-440 SNF is performed on RT-1 facility. Amount of vitrified HLW, which will be returned to Ukraine, is not yet defined. Given estimate of HLW volume is based on the assumption that 1 t of SNF generates 0.15 m^3 of vitrified HLW. This estimate may change in the future.
It is assumed that future reprocessing of WWER-1000 SNF will be performed at the RT-2 facility. SNF from WWER-1000 reactors has been accumulating in interim storage (pound). The time of storage is not defined yet. The amount of vitrified HLW, which will be returned to the Ukraine, is not yet defined. The given estimate of HLW volume is based on the assumptions that: 1) 1 t of SNF generates 0.15 m^3 of vitrified HLW; 2) 13 reactors of this type exist; 3) reactor operation is 30 years. There are plans in the Ukraine to extend the operation lifetime of existing reactors by15 years and to build new reactors. This means that the amount of vitrified HLW after reprocessing of SFN from WWER-1000 reactors may be increased by a factor of 2 to 3.

5 For SNF from WWER-440 reactors the cooling time before reprocessing is appr.30 years. For SNF from RBMK-1000 reactors the cooling time is appr.100 years (designed storage time of a dry interim storage for RBMK-1000' SNF, which is now being under construction within the Chernobyl exclusion area). For SNF from WWER-1000 reactors the cooling time before and after reprocessing is not defined yet (see Note 2)

6 Currently there is very limited information available about RN inventory of BWR SNF from RBMK-1000 reactors and vitrified HLW after processing of LWR SNF from WWER-440 and WWER-1000 reactors [UKR, 2008, Attachment 1].

7 Container type has not yet been defined.

8 Disposal concept and repository layout have not yet been defined.

RN migration parameters	Ref. [1]
References	[1] Justinavičius, D., A. Narkūnienė, P.Poškas, R.Poškas., The Use of Numerical Models in Support of Site Characterization and Performance Assessment Studies of Possible Geological Repository in Clay Formation in Lithuania, Draft Country Report, Feb., 2010. [2] Justinavičius, D., A. Narkūnienė, P.Poškas, R.Poškas. The Data for Far Field Comparison Studies iii (to Ukraine), Kaunas, LEI, 2010 [3] SKB, TR-04-19: Spent fuel performance under repository conditions: a model for use in SR-CAN, SKB, Stockholm, Sweden, 2004. [4] Boguslavskyy, A., V.Shestopalov, Yu. Shybetskyy and B. Stetsenko, Forecast of Radionuclides Migration from Geological Repository at Early Stages of Siting Geological Repository (as Applied to Granitoid Formations of Korostensky Pluton and Chernobyl Exclusion Zone, Ukraine), Contract Report, August, 2008.

Annex III

COMPUTER CODES

AMBER [10][9]: AMBER, developed by Environ and Quintessa, is a flexible graphical-user interface based software tool that allows users to build their own dynamic compartmental models to represent the migration, degradation and fate of contaminants in environmental and engineered systems. AMBER allows the user to assess routine, accidental and long-term contaminant release.

CHETMAD [5]: CHETMAD is a module of the EMOS safety analysis code. It handles advection, diffusion, dispersion and equilibrium sorption in one dimension with diffusion into immobile pore water.

COMPASS: (Code for Modelling Partly Saturated Soil) has been developed by Cardiff University over the last 15 years. COMPASS is a transient finite element code, which can solve problems involving partly saturated soil and ground behaviour. In particular, COMPASS is able to model heat transfer, moisture migration and air transfer, coupled with stress/strain behaviour.

ConnectFlow [18]: ConnectFlow (CONtinuum and Network Contaminant Transport and FLOW) is the suite of Serco Assurance's groundwater modelling software that includes the NAMMU continuum porous medium (CPM) module and the NAPSAC discrete fracture network (DFN) module for modelling groundwater flow and transport in both fractured and porous media on a variety of scales

DUST-MS [6]: The DUST-MS (Disposal Unit Source Term – Multiple Species) computer code is designed to model water flow, container degradation, release of contaminants from the waste form to the contacting solution and transport through the subsurface media.

EMOS [5]: EMOS is a safety analysis code developed by GRS. It can be adapted to model the evolution of a repository both under normal and accident conditions. The package consists of modules that can be used both for deterministic and probabilistic analyses of the integral repository system or of repository subsystems, including the near field, the far field or geosphere, and biosphere.

FEFLOW [7]: FEFLOW (Finite Element subsurface FLOW system) is a computer program for simulating groundwater flow, mass transfer and heat transfer in porous media. The program uses finite element analysis to solve the groundwater flow equation of both saturated and unsaturated conditions as well as mass and heat transport, including fluid density effects and chemical kinetics for multi-component reaction systems.

[9] The references in this annex are with respect to references given in the main text.

GoldSim [4]: GoldSim is a dynamic, probabilistic simulation software developed by GoldSim Technology Group. This general-purpose simulator is a hybrid of several simulation approaches, combining an extension of system dynamics with some aspects of discrete event simulation, and embedding the dynamic simulation engine within a Monte Carlo simulation framework.

GRAPOS1 [5]: It is a module of the EMOS safety analysis code.

MASKOT-K [19]: MASCOT-K is a probabilistic safety assessment code was designed by KAERI based on the MASCOT code designed by SERCO (UK). Each module corresponds to a specific process or barrier and evaluates the corresponding analytical solutions. Unlike the original MASCOT, the MASCOT-K is able to also simulate the SNF dissolution mechanisms. It predicts flux and contaminant concentration at a given time and position.

MODFLOW [25]: MODFLOW is the U.S. Geological Survey modular finite-difference flow model, which is a computer code that solves the groundwater flow equation.

MT3D [26]: MT3D is a 3D solute transport model for simulation of advection, dispersion, and chemical reactions of dissolved constituents in ground-water systems. The model uses a modular structure similar to that implemented in MODFLOW.

MT3DMS [27]: MT3DMS is an extension of MT3D to account for multispecies transport Simulation, in addition to advection, dispersion and chemical reactions of contaminants in ground-water systems.

NAMMU [20]: NAMMU is a finite-element software package for modelling groundwater flow and transport in porous media.

NAPSAC [21]: NAPSAC is the finite-element software package for modelling groundwater flow and transport in fractured rock. A discrete fracture network approach is used to model groundwater flow and the transport of contaminants through the fractured rock.

PORFLOW [8]: PORFLOW is a comprehensive CFD tool developed by Analytic & Computational Research, Inc., ACRi, to accurately solve problems involving transient or steady state fluid flow, heat, salinity and mass transport in multi-phase, variably saturated, porous or fractured media with dynamic phase change.

PMPATH [9,28,30]: PMPATH is an advective transport model running independently from PMWIN [9]. PMPATH retrieves the groundwater models and simulation result from PMWIN and MODFLOW. A semi-analytical particle tracking scheme is used to calculate the groundwater paths and travel times. Both forward and backward particle tracking are allowed for steady-state and transient flow simulations.

TOUGH2 [16]:	TOUGH2 is a general-purpose numerical simulation program for multi-phase fluid and heat flow in porous and fractured media. It is developed in the Earth Sciences Division of Lawrence Berkeley National Laboratory for applications in geothermal reservoir engineering, nuclear waste disposal, unsaturated zone hydrology, and geologic storage of CO_2.

Annex IV

CHINA COUNTRY REPORT

IV-1. INTRODUCTION

The purpose of the simulation studies performed by CPR is to perform deterministic and probabilistic simulations using a highly abstracted representation of the entire geological disposal system (near field and far field) with a TSPA framework using the system-level model GoldSim.

IV-2. GEOLOGICAL DISPOSAL SYSTEM

The geological disposal system consists of the near-field and far-field subsystems. The near-field model is based on the KBS-3 concept, which is illustrated in the LEI progress report [1]; the far field model is based on the UKR semi-generic site (see Annex I) and the related conceptual model described in the third progress report of CPR [2].

IV-2.1. Simplified near-field model

The abstracted near-field model has been set up with nine model blocks, two water blocks representing the void inside the canister and the hole through the canister wall, four blocks representing the bentonite, two blocks representing the crushed rock-bentonite and one for the rock below the deposition hole. Some blocks are further discretized into a total of 19 compartments. The discretization of the near field is presented in Fig. IV-1.

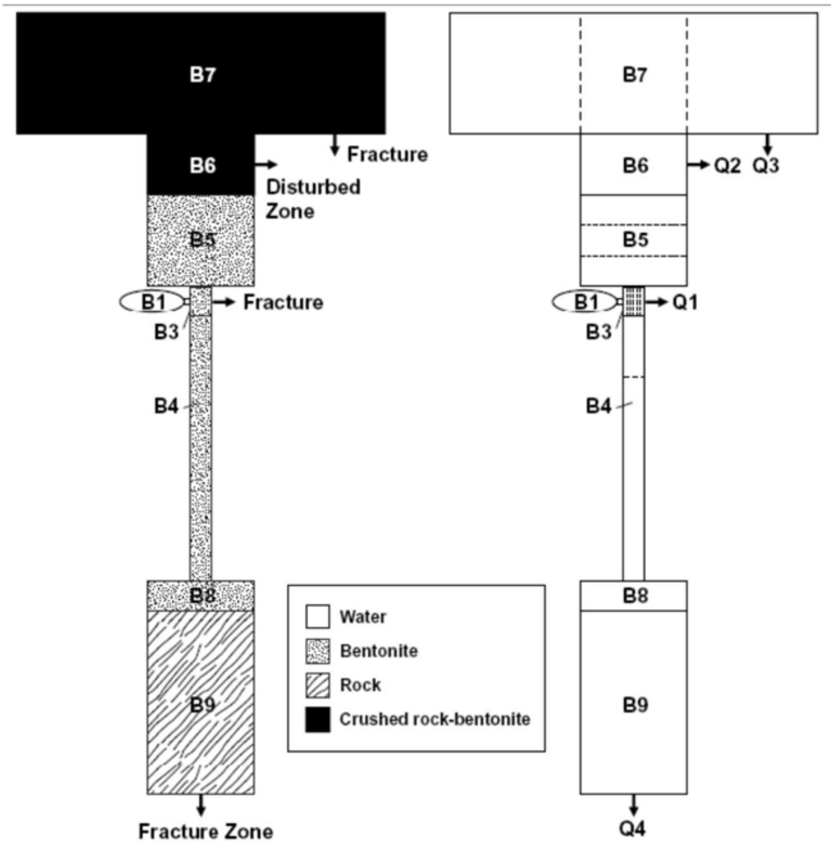


FIG. IV-1. Simplified Near-field Model, left: division of model blocks of the four different materials; right: the subdivision of the model blocks 3, 4 and 7 into compartments.

IV-2.2. Simplified far-field model

The following simplifications are made to represent the far field for TSPA calculations using GoldSim.

(1) The layered formation site is represented by a single porous medium model with a discrete feature (single fault);
(2) The fault is filled with isotropic and homogeneous porous medium;
(3) The fault is priority channel of radionuclide transport by advection and dispersion; radionuclides diffuse into the adjacent matrix;
(4) One-dimensional, steady-state Darcy flow is assumed. The inflow and outflow into priority channel are extracted from UKR's report;
(5) Waste inventory and release rate from the waste canisters are extracted from LEI's report;
(6) Equilibrium sorption according to a linear Henry isotherm is assumed;
(7) Radioactive decay is accounted for.

IV-3. INPUT PARAMETERS

Input parameters used in this GoldSim simulation are taken from the technical report TR-99-23 [3] and LIT's report [1], including geometry, inventory, instant release fraction (IRF), fuel conversion, canister defects and delay time, solubility, sorption, porosity and diffusivity in bentonite and granite and backfill, and parameters in the near and far fields (Tables IV-1 and IV-2).

TABLE IV-1. PARAMETER VALUES USED FOR NEAR FIELD

No.	Parameter	Radionuclide	
		I-129	Se-79
1	Inventory	32 mol/canister	0.028 mol/canister
2	IRF	3	3
3	Solubility	Very high	2.59E-6 mol/m^3
4	K_d in granite rock	0 m^3/ kg	0.001 m^3/ kg
5	D_e in granite rock	8E-15 m^2/s	4E-14 m^2/s
6	Reference diffusivity	1E-9 m^2/s	1E-9 m^2/s
7	Porosity of granite rock	0.005	0.005
8	K_d in bentonite	0 m^3/ kg	0.003 m^3/ kg
9	D_e in bentonite	3E-12 m^2/s	7E-11 m^2/s
10	Porosity of backfill material	0.41	0.41
11	K_d in the crushed zone	0 m^3/ kg	0.001 m^3/ kg
12	D_e in the crushed zone	1E-10 m^2/s	1E-10 m^2/s
13	Porosity of crushed zone	0.3	0.3
14	Flow rate from Q1		9.49E-4m^3/yr
15	Flow rate from Q2		3.16E-3 m^3/yr
16	Flow rate from Q3		3.16E-2 m^3/yr
17	Flow rate from Q4		3.16E-2 m^3/yr

TABLE IV-2. PARAMETERS VALUES AND UNCERTAINTY RANGES USED IN THE SIMULATION OF THE FAR FIELD

No.	Name of Variables	Mean	Min	Max	Standard Deviation	Distribution Type	Remark
1	Fracture Length (km) in the far field	5.505	5.099	6.0	0.2	Normal	Defined by CPR
2	Fracture aperture(m) in the far field	0.1	0.01	1.0	0.015	Lognormal	Defined on RCM2
3	Fracture Width (m) in the far field	5.05	0.1	10.0	3.0	Normal	Defined by CPR
6	Diffusion_I129 (m^2/s) in the far field	4.19E-14	8.00E-16	8.30E-14	\	Uniform	Defined by CPR
7	Diffusion_Se79(m^2/s) in the far field	2.20E-14	4.00E-15	4.00E-14	\	Uniform	Defined by CPR
8	Porosity of Matrix in the far field	0.00264	0.00028	0.005	\	Uniform	Thickness-weighted average
9	Porosity of Fracture in the far field	0.096	0.04	0.152	\	Uniform	Thickness-weighted average
13	Solubility_I129(mol/m^3)	Very high	\	\	\	\	SKB report [3]
14	Solubility_Se79(mol/m^3)	3.30E-06	2.59E-06	4.00E-06	\	Uniform	SKB report [3]
15	Kd_I129(m^3/kg)	0.0	\	\	\	\	SKB report [3]
16	Kd_Se79(m^3/kg)	1.00E-03	2.00E-04	1.80E-03	\	Uniform	SKB report [3]

IV-4. SIMULATION RESULTS

IV-4.1. Deterministic simulations

Deterministic simulations of ^{79}Se and ^{129}I transport through the near and far fields in porous medium and a discrete fracture have been performed using GoldSim. Figs IV-2 and IV-3 show the normalized cumulative release rate curves (defined as the cumulative activity in the river/well divided by initial activity in canister for ^{129}I and ^{79}Se) for the fracture and the matrix. As expected, the non-sorbing ^{129}I moves faster than ^{79}Se, with most of the radionuclides flowing through the fracture domain.

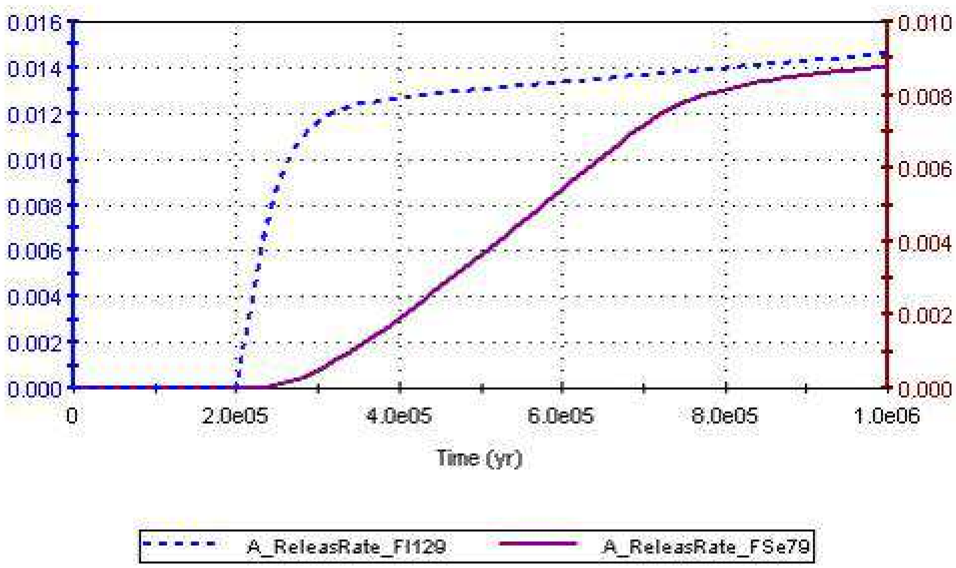


FIG. IV-2. Normalized cumulative release rate through fracture zone to river/well.

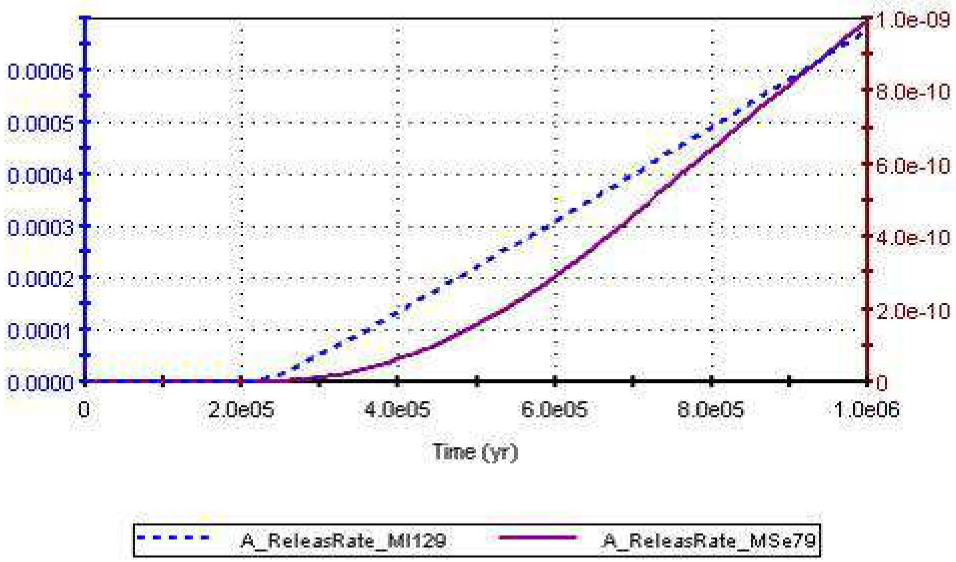


FIG. IV-3. Normalized cumulative release rate through matrix to river/well.

IV-4.2. Sensitivity analysis

The sensitivity analysis is commonly used in performance assessment to determine the degree to which uncertain parameters affect performance-relevant output variables. The geological characteristics can be directly or indirectly represented by the geological parameters in a sensitivity analysis.

GoldSim provides the ability to carry out sensitivity analyses. After specifying input parameters and output variables, GoldSim runs the model multiple times, varying one independent variable at a time through a range of values (Lower Bound, Central Value and Upper Bound) while holding all of the other variables constant. Sensitivity plots reveal the variables in the model to which the results are most sensitive.

For stochastic variables, we often use quantiles to define the range. The Central value is always the 50% percentile. The lower and upper bounds are determined by the number of sampling points for each variable using the following equations:

Lower Bound = 100%/(No. of Points*2); Upper bound = 100%-Lower Bound.

For deterministic variables, the range must be specified directly.

In this report, the result we would like to analyse for sensitivity is the peak value of normalized cumulative release rate. The selected nuclides are ^{79}Se and ^{129}I.

There are about 10 variables selected for sensitivity analysis, as listed in Table IV-2. The range of each independent variable is defined (see Table IV-3).

TABLE IV-3. SELECTED VARIABLES FOR SENSITIVITY ANALYSIS

No.	Name of Variables	Units	Lower Bound (%)	Central Value (%)	Upper Bound (%)
1	Fracture Aperture	Mm	16.7	50	83.3
2	Fracture Width	M	16.7	50	83.3
3	Fracture Length	M	16.7	50	83.3
4	Porosity of Fracture Zone	-	16.7	50	83.3
5	Porosity of Matrix	-	16.7	50	83.3
6	Flow Rate	m^3/s	16.7	50	83.3
7	Solubility	mol/m^3	16.7	50	83.3
8	Kd in Matrix	m^3/kg	16.7	50	83.3
9	Kd in Fracture Zone	m^3/kg	16.7	50	83.3
10	IRF	-	16.7	50	83.3

A tornado chart is used to display the results of the sensitivity analysis. The tornado chart shows the ranked sensitivity of the selected results to the independent variables. In the tornado chart, each bar represents the range of results produced when each independent variable is set to its lower bound, central value and upper bound. In the following figures, a light blue bar indicates that the value was produced by the lower bound, and a dark blue bar indicates that the value was produced by the upper bound.

In order to better visualize the relative sensitivity of the independent variables, the variables listed in Table IV-3 are divided into three groups: 1) geometric parameters of near- and far field, i.e. fracture aperture, fracture width, fracture length and porosity; 2) transport parameters, i.e., solubility, Kd and diffusion coefficients; and 3) dissolution parameters of the waste, i.e., IRF and fuel dissolution rate.

The peak value of normalized cumulative release rate is selected as the objective of the sensitivity analysis.

Sensitivity analysis for ^{79}Se

The tornado charts for ^{79}Se are shown in Figs IV-4 to IV-7. The tornado chart of all independent variables is (Fig. IV-4) shows that solubility and Kd in the bentonite are the key parameters affecting the peak value of the cumulative release curve. All remaining parameters have significantly lower sensitivities; the X-axis of the related Tornado charts (Figs IV-5 to IV-7) are rescaled to reveal the relative sensitivity of these parameters.

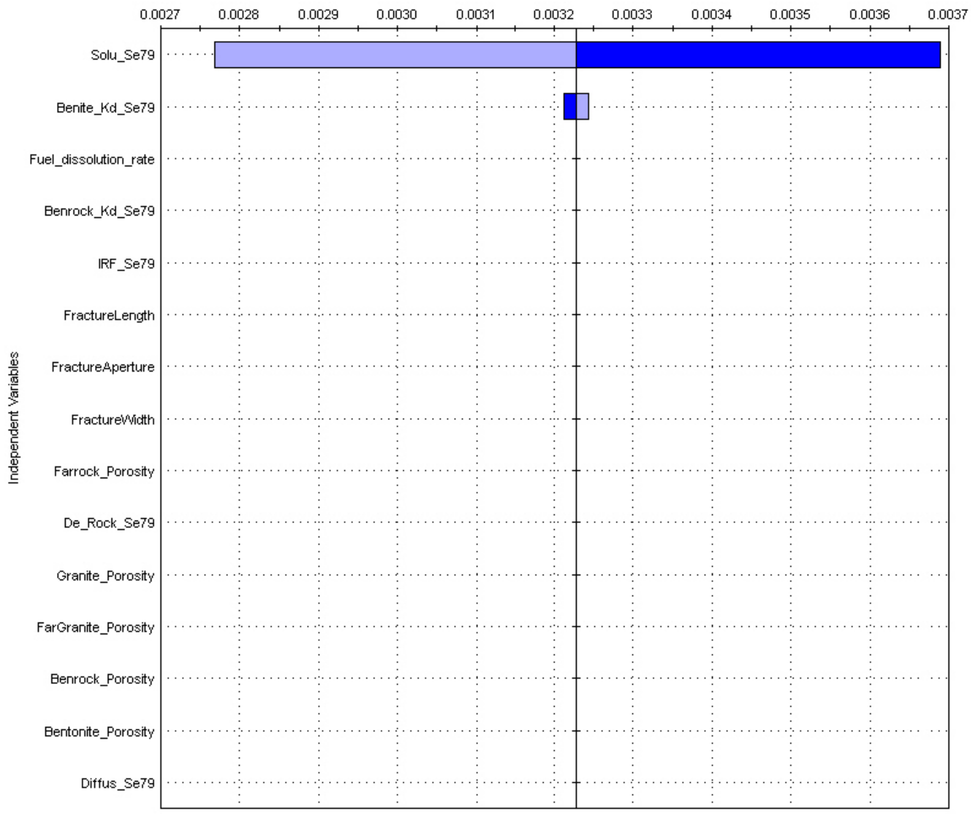


FIG. IV-4. Tornado sensitivity chart of the release rate of ^{79}Se for all variables.

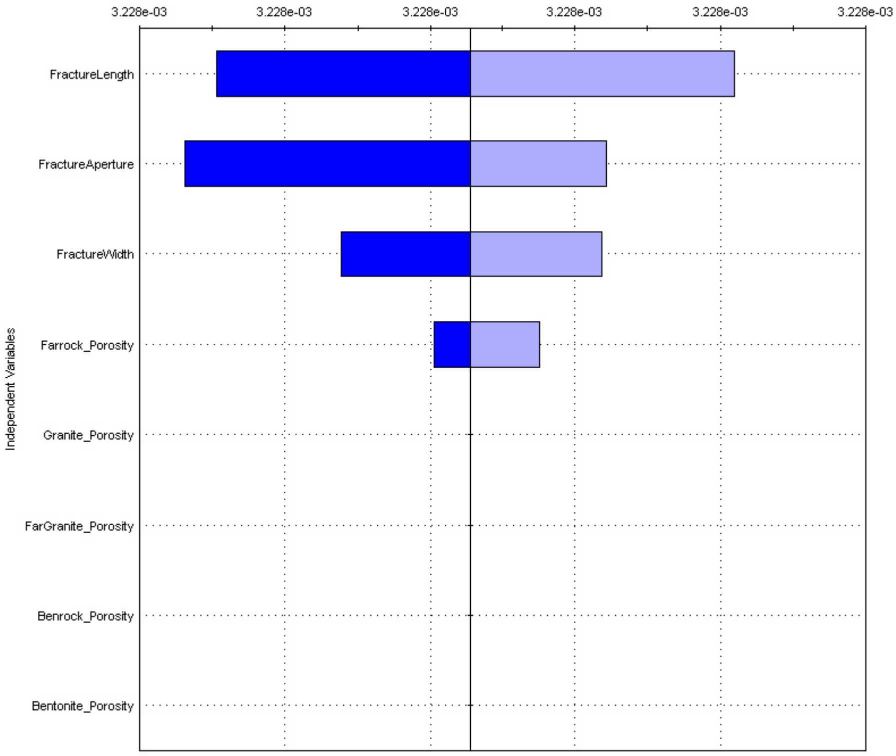


FIG. IV-5. Tornado sensitivity chart of the release rate of ^{79}Se for all geometric parameters.

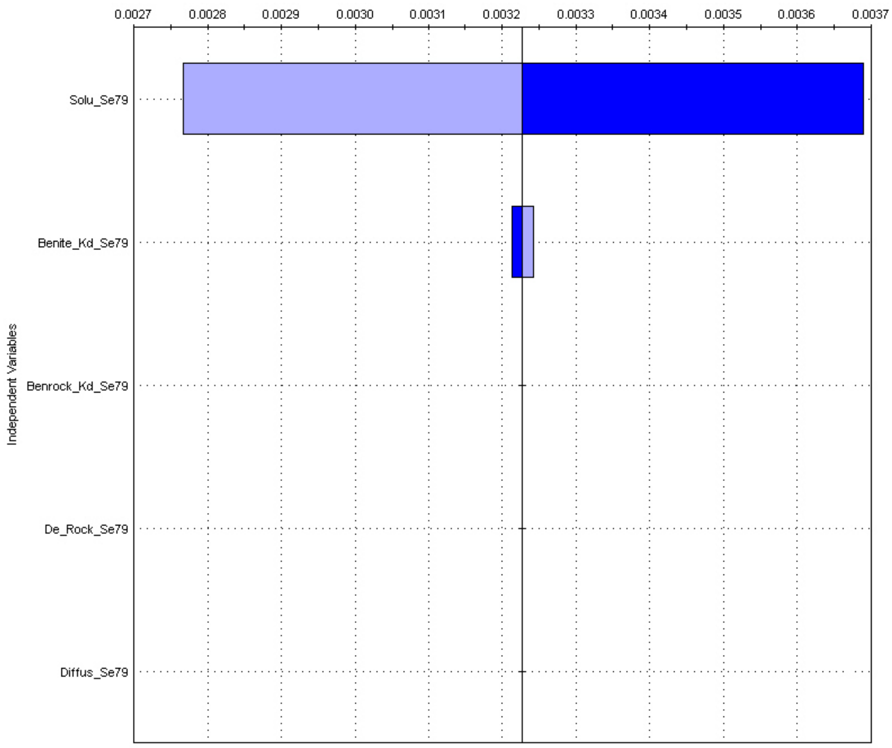


FIG. IV-6. Tornado sensitivity chart of the release rate of ^{79}Se for all transport parameters.

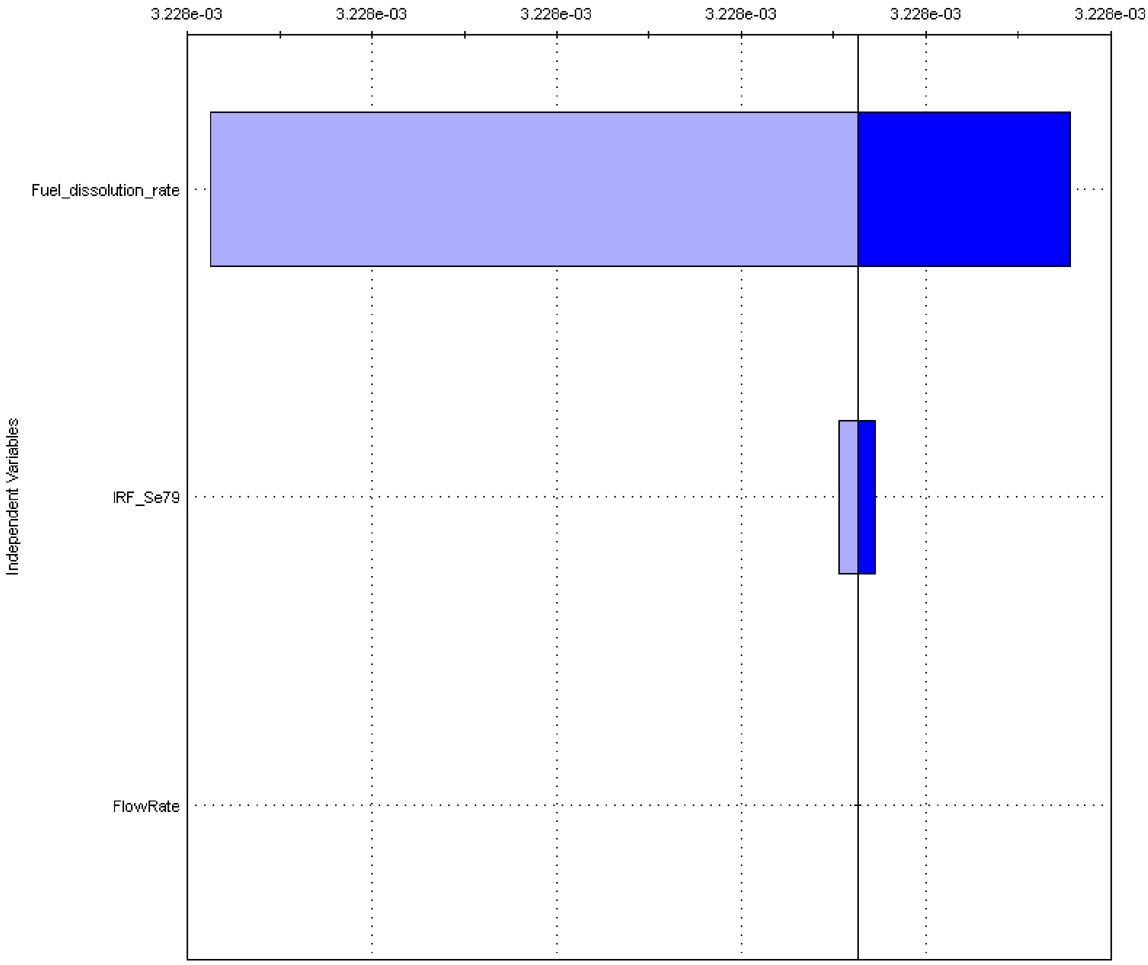


FIG. IV-7. Tornado sensitivity chart of the release rate of ^{79}Se for dissolution parameter. Sensitivity Analysis for ^{129}I.

The tornado charts for ^{129}I are shown in Figs IV-8 and IV-9, showing that the fuel dissolution rate is by far the most sensitivity parameter, followed by the instant release fraction. The other variables are less sensitive, with fracture length and aperture being the most sensitive geometric parameters.

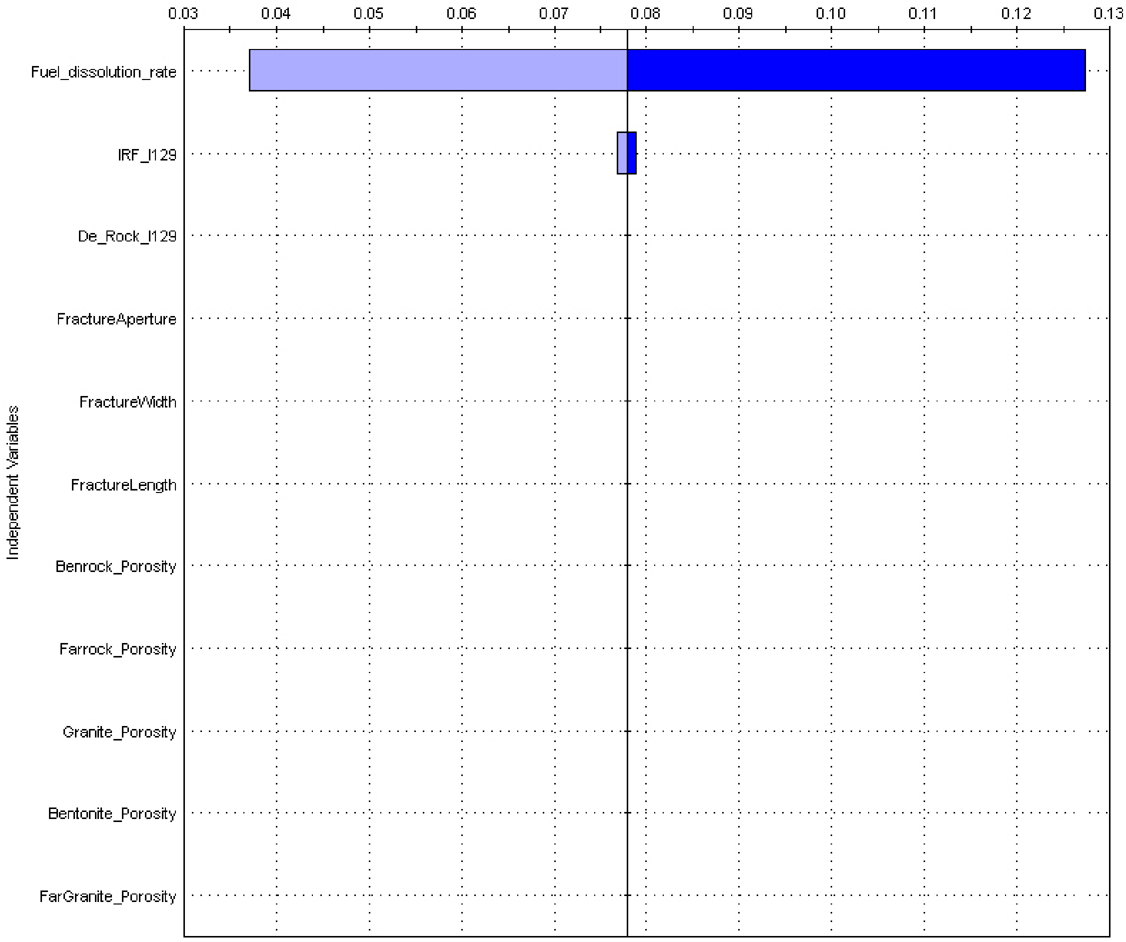


FIG. IV-8. Tornado sensitivity chart of the release rate of ^{129}I for all variables.

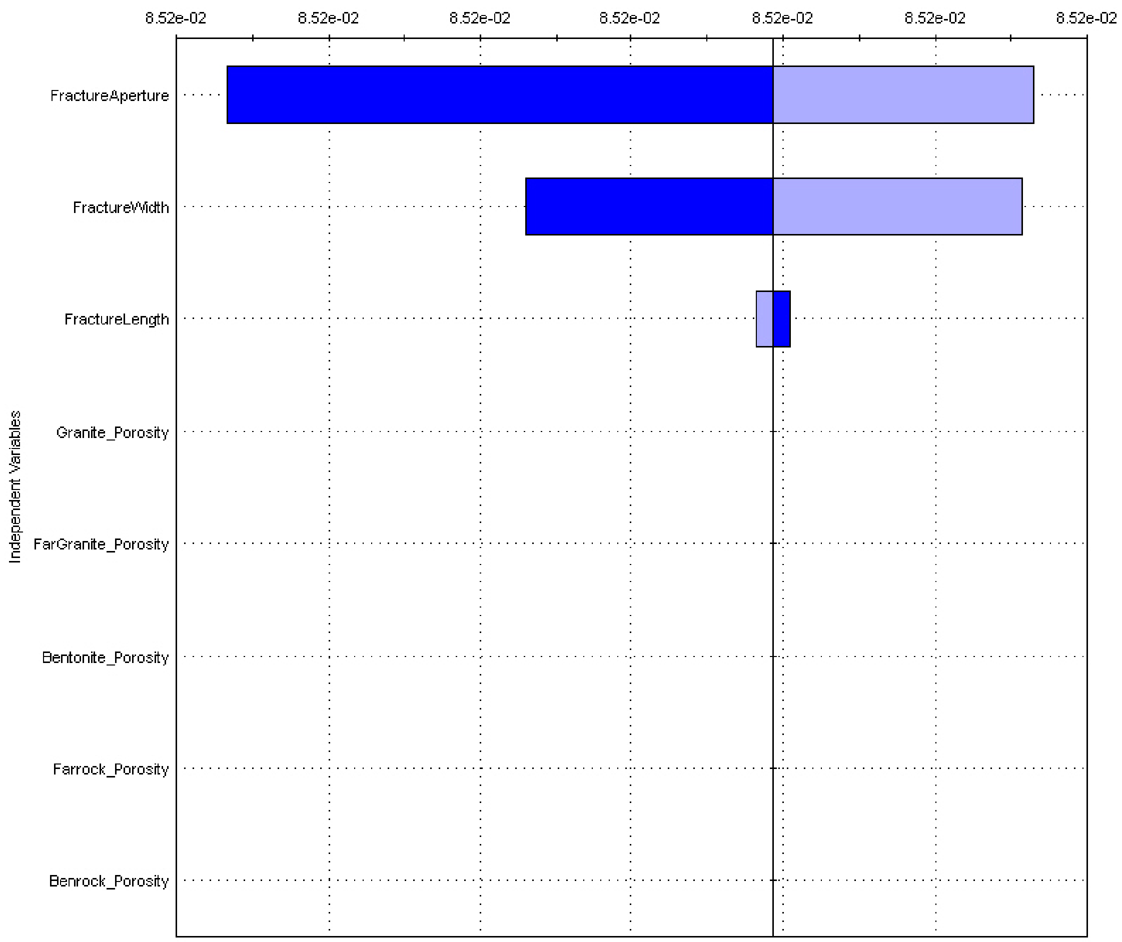


FIG. IV-9. Tornado sensitivity chart of the release rate of ^{129}I for geometric parameters.

The results of the sensitivity analysis have to be interpreted considering the assumptions and simplifications of the near- and far-field models. We assume that pure diffusion is the mechanism of mass exchange between the near and far fields; advective and dispersive transport is negligible because of the very low permeability of the host rock and the very small hydraulic gradient in the geological disposal system.

IV-4.3. Probabilistic simulations

In the probabilistic simulations of the transport of ^{129}I and ^{79}Se, the following six parameters are considered uncertain: Instant release fraction (IRF), solubility, porosity, sorption, geometry of the fracture domain, and water flow rate. Uncertainty distributions were defined for these six parameters, and 50 Monte Carlo realizations were examined to a simulation time of 1 million years. The results are shown in Figs IV-10 to IV-13.

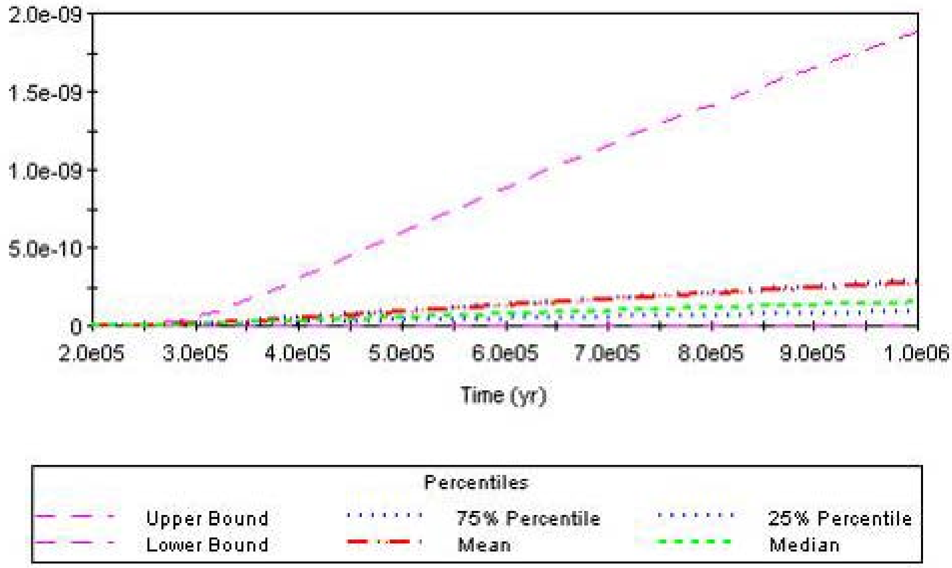


FIG. IV-10. Probabilistic results of cumulative release rate for ^{79}Se in matrix domain.

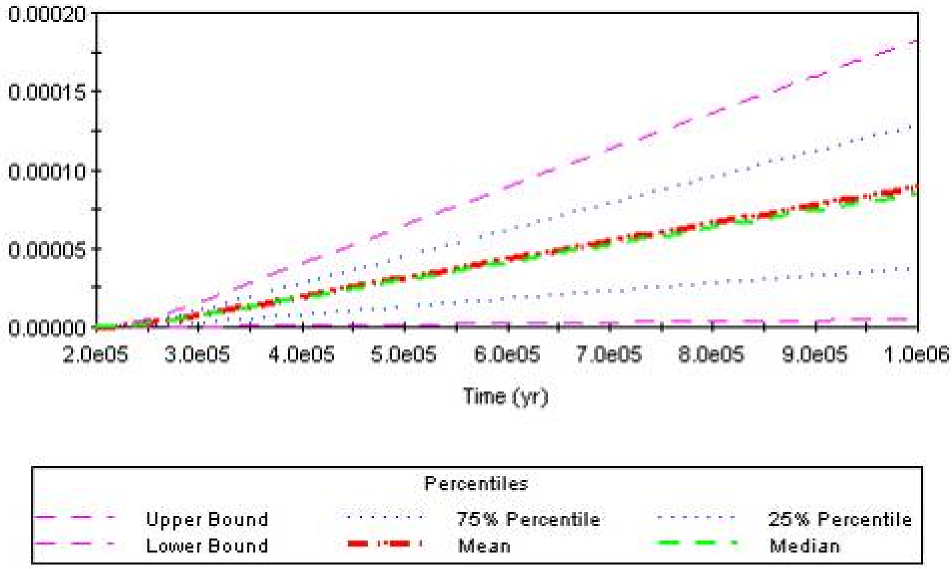


FIG. IV-11. Probabilistic results of cumulative release rate for ^{129}I in matrix domain.

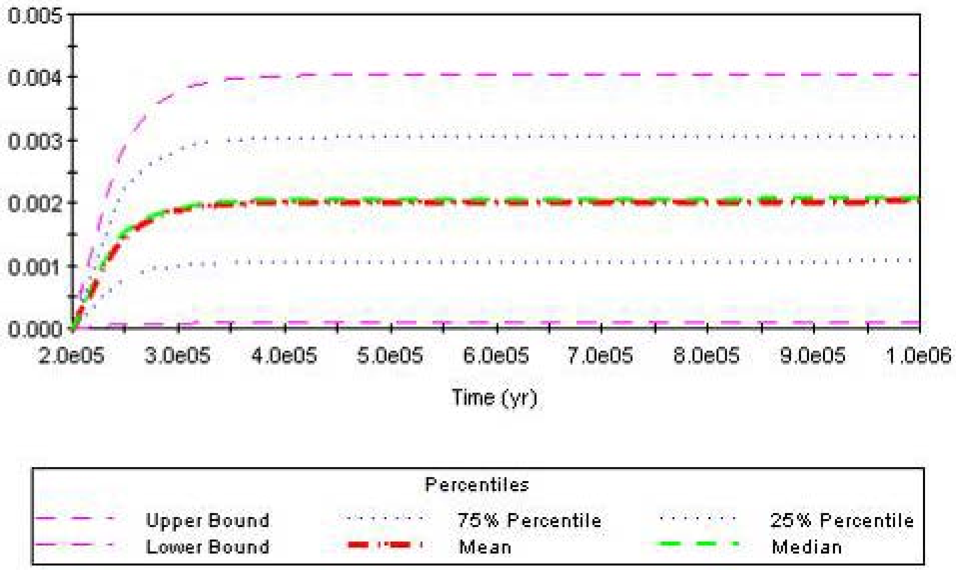


FIG. IV-12. Probabilistic results of cumulative release rate for ^{129}I in fracture domain.

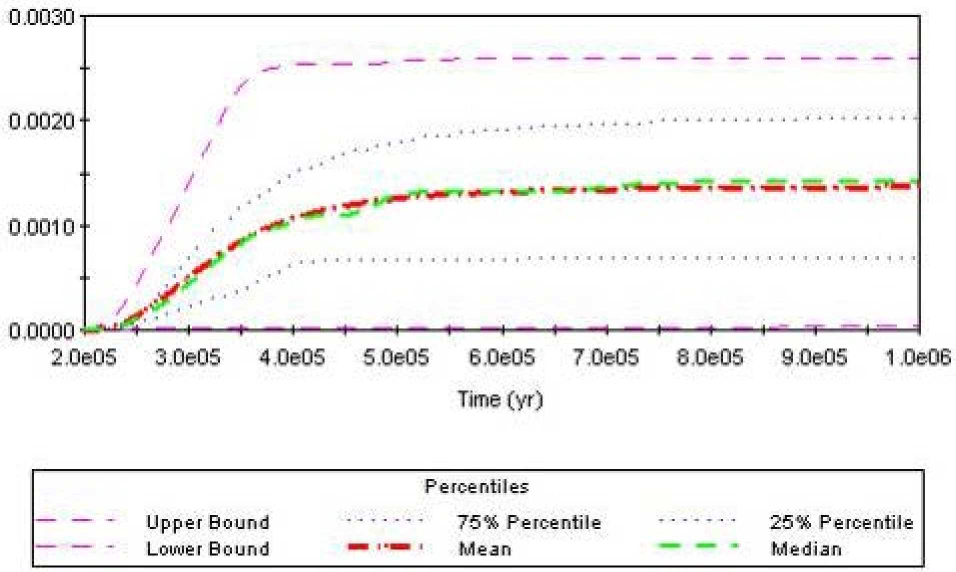


FIG. IV-13. Probabilistic results of cumulative release rate for ^{79}Se in fracture domain.

IV-5. CONCLUSIONS

The project can be summarized as follows:

(1) We built a preliminary GoldSim TSPA model that represents a geological disposal site. This framework is useful for the future research work of TSPA of China's geological disposal system;
(2) The expertise gained in using Goldsim is considered useful for future site characterization studies, the design of laboratory experiments and field activities;
(3) A group specialized in numerical modelling has been established. This is a very important outcome of this project, supporting the on-going programme of siting and site characterization of a geological repository in China;
(4) It is recognized that this preliminary TSPA framework is just an exercise, and in no way represents a real TSPA model to be developed for the assessment of China's geological disposal system.

References to Annex IV

[1] BRAZAUSKAITĖ, A., POŠKAS, P., POŠKAS, R., The Use of Numerical Models in Support of Site Characterization and Performance Assessment Studies of Possible Geological Repository in Clay Formation in Lithuania, Country Report, Kaunas, 2008.
[2] SU, R., CHEN, W., ZONG, Z., ZHOU, J., Sensitivity Analysis and Uncertainties Simulation of CRP-GEORC Model by GoldSim Code, Progress Report (III), 2008.
[3] LINDGREN, M., LINDSTRÖM, F., Radionuclide transport calculations, TR-99-23, December 1999.

Annex V

LITHUANIA COUNTRY REPORT

V-1. INTRODUCTION

This report summarizes the major activities performed during the past five years and represents essential results achieved by the LIT team.

In the beginning of the project, two types of geological formations (crystalline rocks and clay formations) for the disposal of the SNF were being analyzed. Moreover, two different types of SNF (BWR SNF and RBMK-1500 SNF) were taken into account. Later in the project, only conceptual models in crystalline rocks and geological disposal of RBMK-1500 SNF were analyzed.

The final country report summarizes the research activities, which includes (1) the assessment of radionuclide transport in the near-field region of a spent nuclear fuel (SNF) repository, (2) groundwater flow and radionuclide transport analysis in the far-field region, and (3) numerical modelling of the coupled processes in the near-field region.

V-2. NEAR FIELD MODELLING

For the assessment of the radionuclide release from the near-field region of the repository, an integrated finite difference method and the concept of compartments was applied. For the numerical simulation of the radionuclide transport, the computer code AMBER 4.5 has been chosen. The deterministic analysis considers a vertically emplaced waste canister; the probabilistic analysis considers a horizontal configuration. The respective discretization of the near field is presented in Fig. V-1.

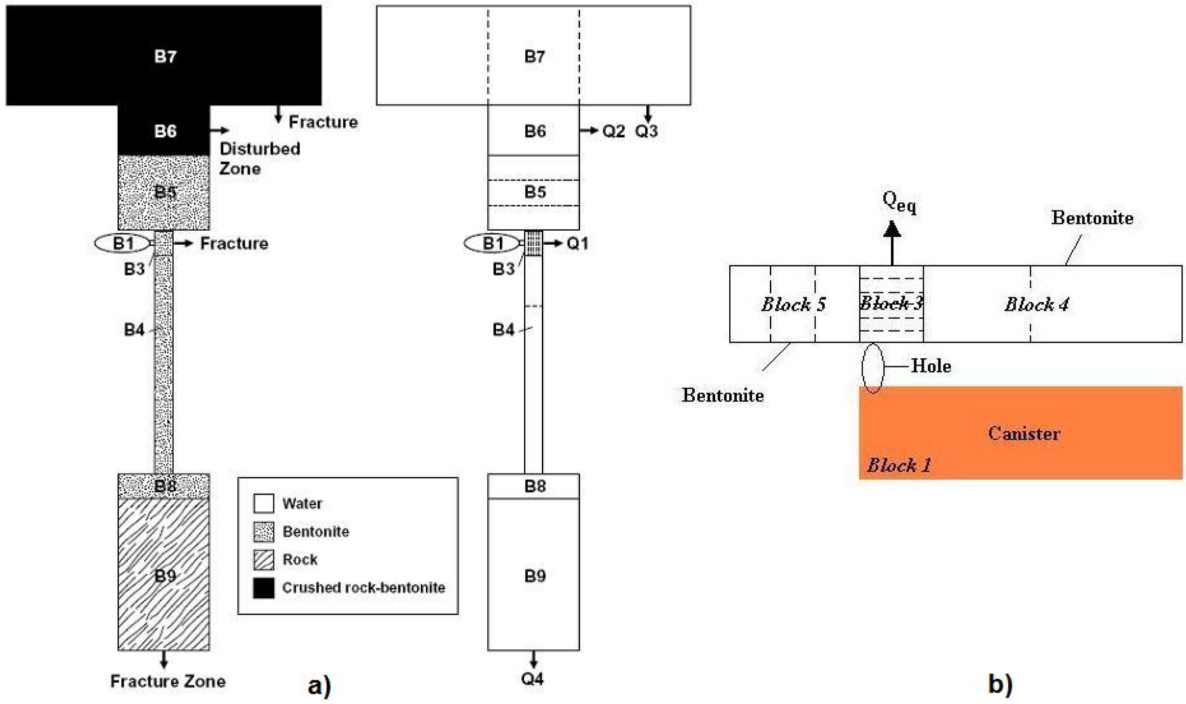


FIG. V-1. Schematic of the near field compartment model for the (a) KBS-3V concept, and the (b) KBS-3H concept.

A simulation of the radionuclide release from the near field of a KBS-3 type disposal system with the disposal canister loaded with 32 half-assemblies of RBMK-1500 SNF was performed. The radionuclide transport analysis was assessed for the RBMK-1500 SNF with initial enrichment of 2.8% U-235 and 0.6% Er_2O_3. The SNF burnup is approximately 29 MWd/kgU. The radionuclide inventory was assessed by computer code SAS2H (computer code system SCALE 5).

A single canister-defect scenario was chosen for the deterministic analysis of near-field releases. The probabilistic analysis of radionuclide migration was expanded, including various canister defect and climate-change scenarios. The main assumptions of the scenarios, the parameters values, and related references can be found in full report [1].

The deterministic and probabilistic analyses (see Fig. V-2) of different scenarios consistently showed that the radionuclides dominating near-field releases are Ni-59, Nb-94, I-129, Cs-135 and Ra-226. At longer times, the release is dominated by Ra-226, a naturally occurring radionuclide, which is formed by ingrowth from the decay chain of U-238. Ra-226 is a more mobile radionuclide, which thus is transported faster through the near-field region than its parent radionuclides.

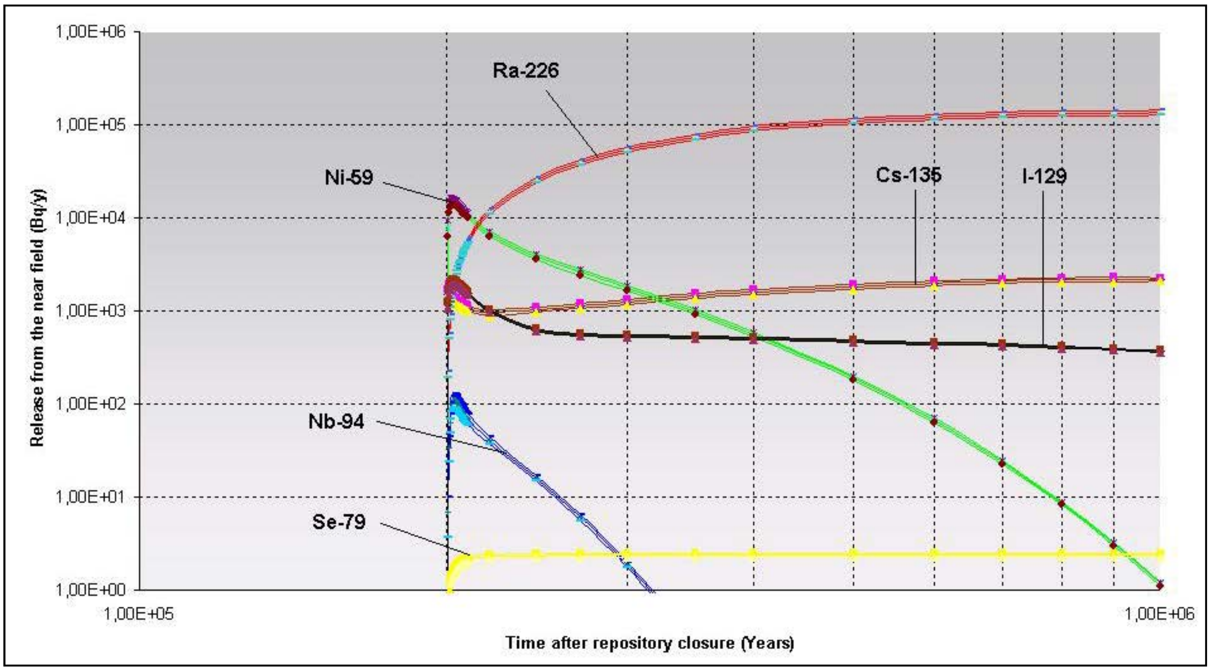


FIG. V-2. Probabilistic assessment of near-field releases for scenario A.

The releases from the near field of Se-79 and I-129 under different scenarios are presented in Figs V-2 and V-3. The mean releases rate from a probabilistic assessment is higher than those from the deterministic analysis for the radionuclides analyzed. The largest increases of the maximum release rate were observed for the Nb-94 and U-238 decay chains; the smallest increases were observed for Ni-59 and Se-79.

The results of the probabilistic analysis show that due to the uncertainty related to the defect growing time the confidence limits for the mean releases tend to be wider at the beginning for some nuclides such as Ni-59, Nb-94 and I-129. It is also observed that the uncertainty in the canister defect growing time has a major impact on the maximum mean release of Nb-94 and has no significant influence on the maximum release of the other radionuclides being analyzed.

Comparative analyses of the radionuclide releases from the near field under different scenarios have shown that the profiles of the release curves and maximum release rates are different. This is a result of different canister defect evolution, different modelling assumptions, and different parameter values.

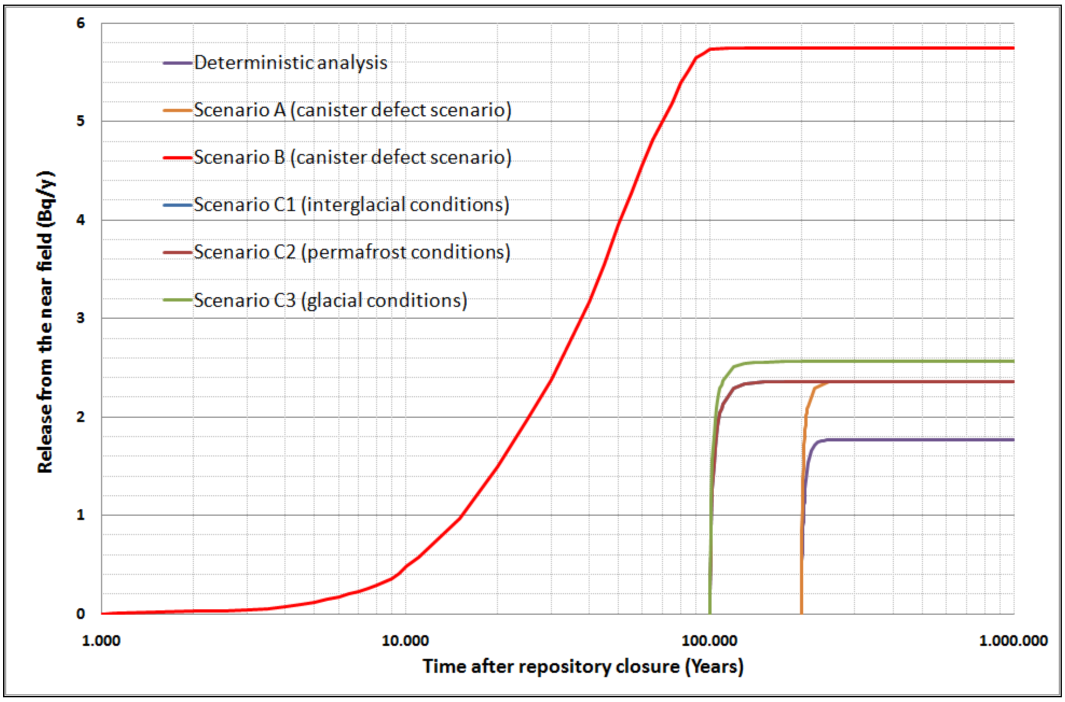


FIG. V-3. Release of Se-79 from near field region for different scenarios.

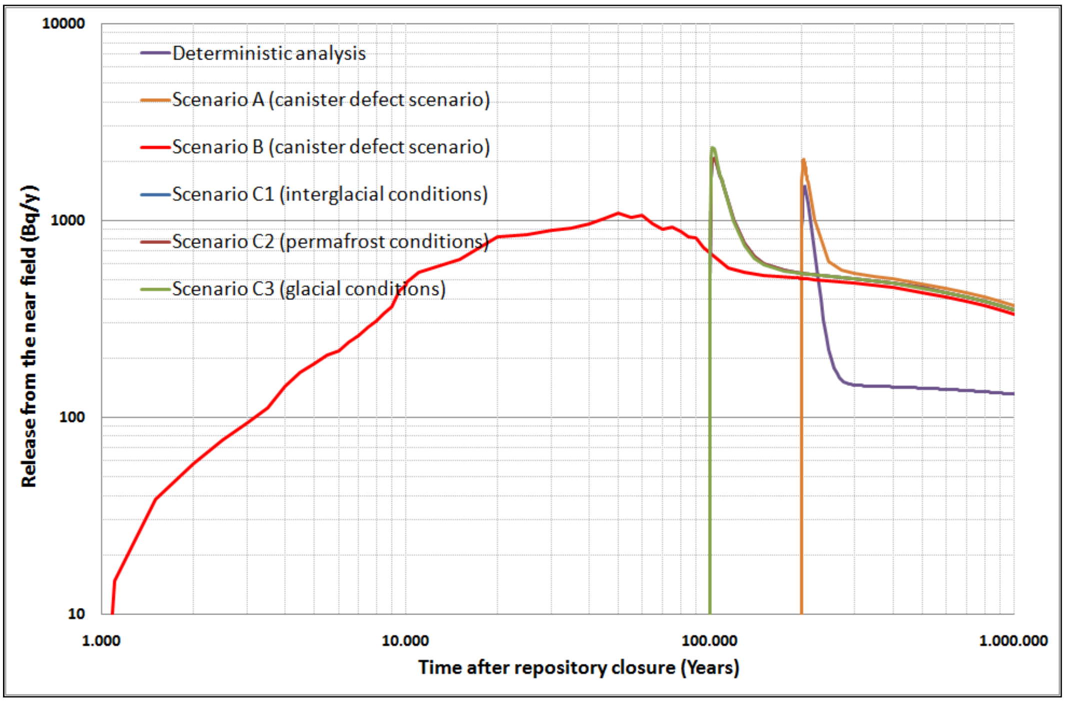


FIG. V-4. Release of I-129 from near field region under different scenarios.

Figs V-3 and V-4 demonstrate that the deterministic analysis shows a lower release rate from the engineering barriers compared to the probabilistic analysis. This could be related to the pessimistic parameter values used in the probability distribution function (these value leads to the highest release rates). The releases considering conditions typical for the interglacial and permafrost periods are equal for Se-79 and I-129, because in the case of highly saline pore water in the bentonite buffer, the release does not depend on the sorption behavior for of weakly and non-sorbing radionuclides (such a Se-79 and I-129). The highest maximum release of Se-79 is for Scenario B (canister defect at varying times between 1000 and 100,000 years), and the highest maximum release of I-129 is obtained if assuming glacial conditions.

The analysis was also performed using parameters defined for the base case of the comparison study. The radionuclide release from the near field in normalized form were compared with the results of other modelers in order to evaluate the sensitivity of the release rates to the conceptual model, computer code, and the disposal concept. Good agreement of the normalized cumulative release of the selected radionuclides was observed with the results of other modelers showing low sensitivity of the results to computer code and its numerical scheme, geometry of the near field, and initial inventory.

V-3. FAR FIELD MODELLING

For the modelling of groundwater flow and radionuclide transport, a porous medium approach was applied. The conceptual model was based on the initial data provided and the schematization of the hydraulic properties for 2D hydrogeological model of Veresnia (Ukraine) site. The TOUGH2 code was used.

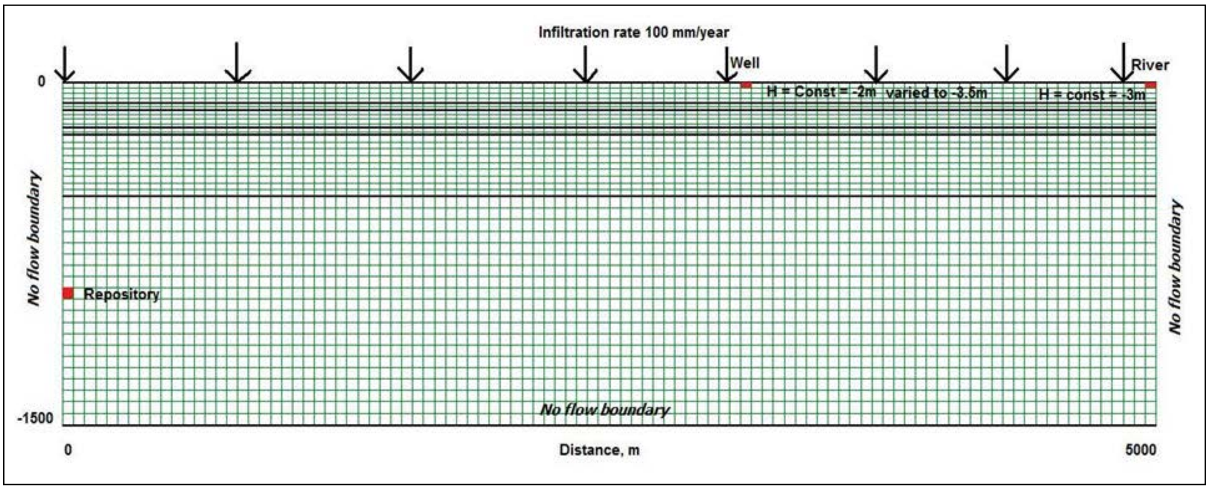


FIG. V-5. Conceptual model of the Veresnia site and TOUGH2 model grid.

The long-lived radionuclide, I-129, was chosen as the reference radionuclide for the analysis of radionuclide transport in the far field. A particular amount of I-129 was injected at the source into a steady-state groundwater flow field. The time dependent injection curve of I-129 was based on the results of the probabilistic analysis of near-field release. The conceptual model was adapted for three different scenarios.

Two different cases of horizontal groundwater flow regime have been analysed (with and without consideration of the groundwater flow due to regional head gradient). The comparison of the results (see Fig. V-5) shows that including regional groundwater flow (0.1% head gradient) leads to an earlier and higher maximum release of I-129 into the river compared to the “no regional flow” case:

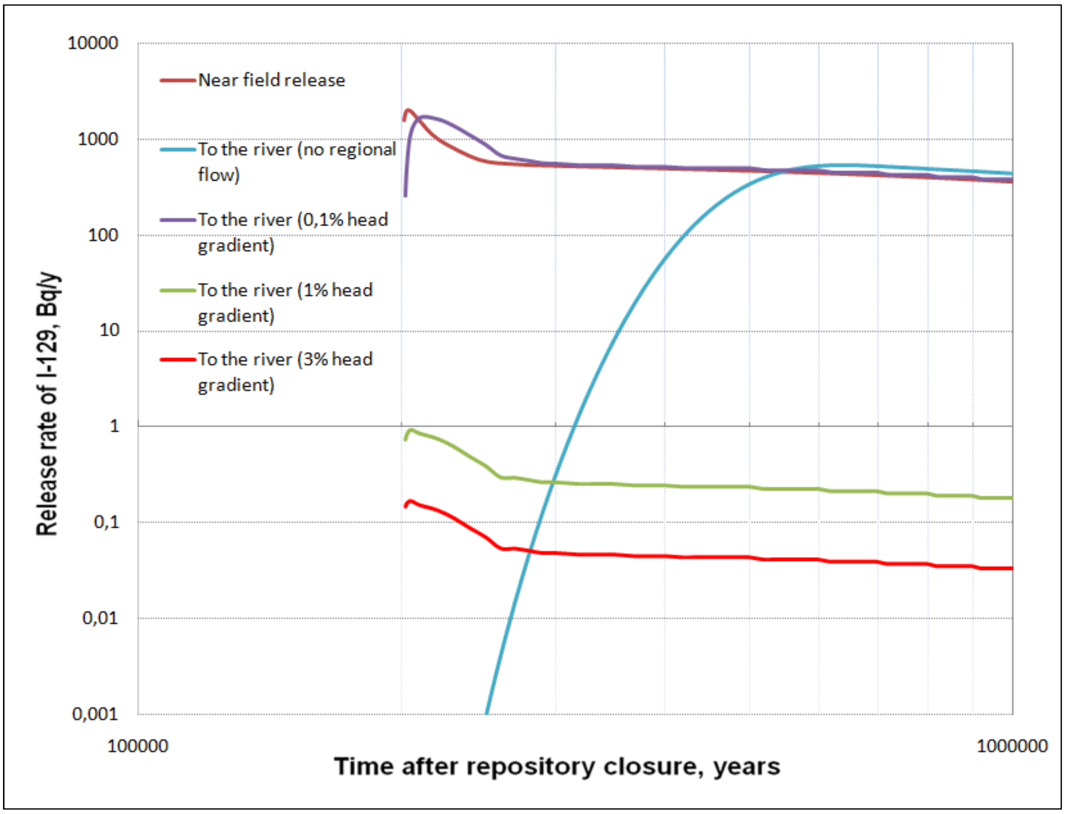


FIG. V-6. Release of I-129 from the far field under regional flow conditions with different head gradients.

If there is no regional groundwater flow, the influence of different well discharge rates (keeping constant level drawdown in the river) on the groundwater flow regime (and radionuclide migration in the far field) was investigated. The results show that different internal head drawdown in the discharge point greatly influence the groundwater flow regime, and thus lead to different release rates of radionuclide at the discharge points.

The ratio between the maximum release rate from the far field and from the near field indicated that the maximum rate of radionuclide release to the river is lower than the maximum release rate from the engineered barriers in all cases being analyzed.

The comparative analysis of the radionuclide releases into the river under different scenarios shows that the profiles of the release curves and maximum release rates are different. The main discrepancy between the permafrost and glacial scenario is that different permafrost depths (500 m and 90 m, respectively) are expected. Under glacial conditions, the groundwater from the sedimentary cover influences the discharge of the groundwater into the river from the upper geological layers. Under permafrost conditions, the groundwater must be pumped from the deeper geological layers due to frozen groundwater in the sedimentary cover (upper layers), which leads to larger release of I-129 into the river under permafrost conditions.

Comparative analysis of the groundwater flow and radionuclide transport using the porous medium approach showed that the results correlate quit well with the results of UKR.

V-4. COUPLED PROCESS MODELLING

Two coupled processes have been investigated: thermal-hydrological (TH) and thermal-hydrological-mechanical (THM). TH effects were simulated to address the question whether heat generation from the waste canister and gas generation due to canister corrosion would influence radionuclide transport from the near field into the fractured rocks surrounding disposal canisters. The modelling results using TOUGH2 are shown in Fig. V-7, which indicates that the coupled processes in the near field may affect radionuclide release rates, especially at the beginning of the release. Therefore, coupled effects should be taken into consideration.

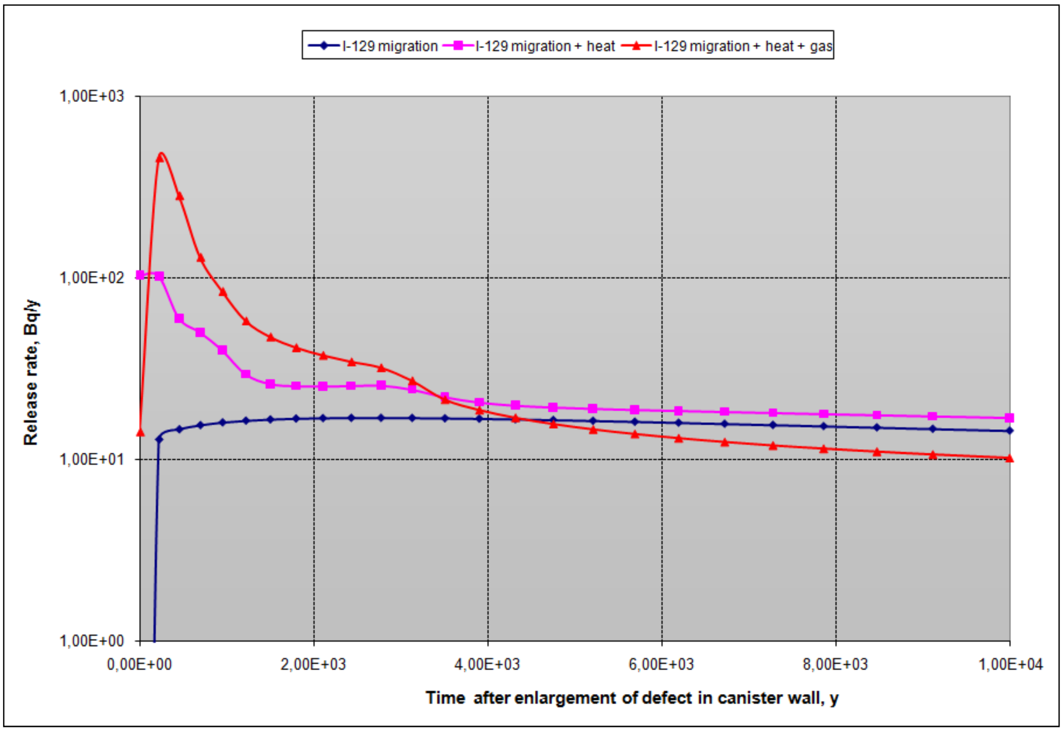


FIG. V-7. I-129 release from the bentonite barrier to the fracture at fracture opening.

The numerical investigation of the behavior of engineered barriers taking into account THM processes was performed using the COMPASS code. Fig. V-8 shows the conceptual model, which represents the KBS-3V disposal concept.

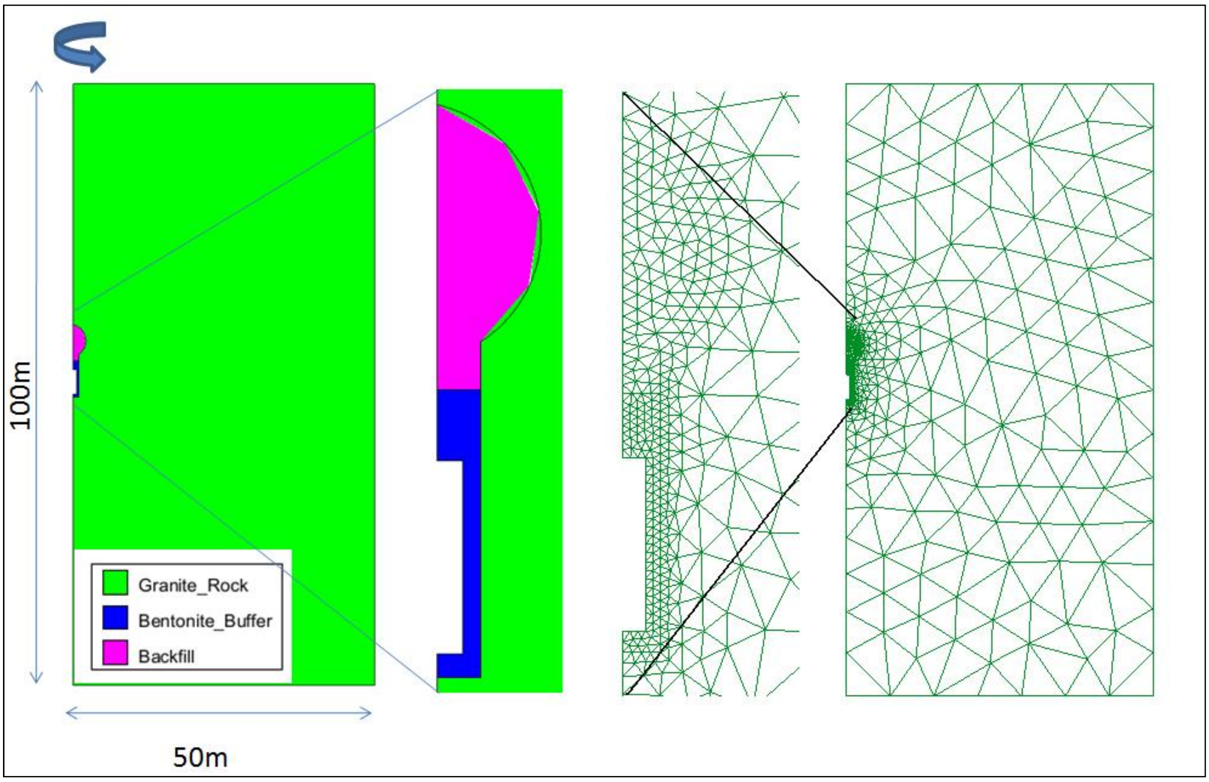


FIG. V-8. Schematic view of conceptual model to estimate coupled THM processes.

The evolution of temperature, saturation and stresses in the bentonite buffer was calculated. The modelling results summarized in TABLE V-1 indicate that the maximum temperature is slightly higher if coupled TH and THM processes are taken into account, as compared to a purely thermal (T) analysis where the coupling of temperature changes and hydro/mechanical processes is ignored. The character of the thermal evolution in the T and TH analyses correlate quit well with those obtained by ROM. Differences are likely due to different inventories, initial and boundary conditions, and material properties.

TABLE V-1. CALCULATED MAXIMUM TEMPERATURE AT MONITORED POINTS

	T analysis	TH analysis	THM analysis
P1	309.6	309.8	309.8
P2	332.9	333.4	333.6
P3	321.6	321.9	321.8
P4	311.1	311.3	311.2
Maximum temperature	333.1	336.4	336.3

According to the modelling results, the maximum temperature in the system was observed to be 336.4 K. There is a requirement that the surface temperature of the canister may not exceed 100˚C. The results of the temperature assessment around the canisters loaded with 32 RBMK-1500 SNF half-assemblies showed that a disposal canister with such a heat output would satisfy the temperature constrain.

The TH and THM analysis gave very similar results on the re-saturation time of the near field rock and bentonite, while the analysis without taking into account the coupling of the processes showed a shorter re-saturation time of the near-field rock, and longer time for bentonite.

TABLE V-2. RE-SATURATION TIMES OF DIFFERENT MATERIALS IN H, TH AND THM ANALYSIS

	Near field rocks	Bentonite*	Backfill
H analysis	18.5 y	19 y	> 200 y
TH analysis	6.5 y	38 y	> 200 y
THM analysis	6.5 y	37.5 y	> 200 y

* With the exception of the area close to the canister

The assessment of the mechanical displacement showed that the vertical displacement scale contains values up to 3 times higher than the horizontal displacement. The results obtained indicate the importance of the coupled processes analysis for more realistic assessment of the disposal system behavior.

Reference to Annex V

[1] JUSTINAVIČIUS, D., NARKŪNIENĖ, A., POŠKAS, P., POŠKAS, R., The Use of Numerical Models in Support of Site Characterization and Performance Assessment Studies of Possible Geological Repository in Clay Formation in Lithuania. Draft Country Report, February 2010.

Annex VI

ROMANIA COUNTRY REPORT

VI-1. INTRODUCTION

VI-1.1. Background

The Romanian team performed one-dimensional source-term modelling and one- and two-dimensional modelling of the far-field groundwater flow and contaminant transport. Radiological dose estimates to humans were obtained for the 1D modelling of the repository system. Romania proposed a repository concept, based on the Canadian concept, which was modelled as a 1D source term with the codes GRAPOS1 (a module of the German assessment code EMOS) and DUST-MS. Romania proposed two types of simulations: Two-dimensional FEFLOW modelling of flow and transport in porous and fractured media, as well as a one-dimensional far-field modelling with CHETMAD, a component of the EMOS code. The influence of the source-term boundary conditions on contaminant fate was investigated, using one-dimensional simulation of the near field with DUST-MS, and two-dimensional flow and transport calculations with PORFLOW.

VI-1.2. Objectives

The work performed by the Romanian team aimed at demonstrating the influence of the modelling assumptions on simulated release from the near field, as well as on groundwater flow and contaminant transport in the far field. Coupled thermal-hydrologic process simulations are initiated.

VI-1.3. The near-field model

The source term is influenced by the local flow conditions, and considers mobilization of contaminants after container failure, instantaneous release of the inventory in the fuel gap and concurrent release of the contaminants from the fuel matrix and metallic parts. The mobilized inventory, subjected to solubility limits in the volume of dissolution inside the container, diffuses into the buffer, reaching the excavation disturbed zone (EDZ), which is intersected by water-conducting zones. Radionuclides are transported advectively from the EDZ towards the biosphere.

VI-1.4. The far-field model

The computation is restricted to a two-dimensional cross section (5000 m × 1200 m) of the disposal site. The model includes a sedimentary cover having two aquifers, separated by an aquitard and the granite layer which is separated from the lower aquifer by a second aquitard. Two layers can be distinguished in the granite: an upper part, the *fractured granite* and the lower part, the monolithic granite where the repository is located.

VI-2. APPROACH

VI-2.1. The near-field model

The first type of simulations considers the repository located in a porous media. The flow field in the geological formation influences the transport of contaminants released from the boundary between the repository EDZ and the host rock.

In a second iteration, the repository is considered to be intersected by a fracture that crosses the geological environment. The fracture crossing the disposal boreholes influences the flow of water in the EDZ. Two values have been assigned for the fracture aperture: 0.1 mm and 1 mm. As a consequence, the flow of water in the EDZ of the disposal boreholes changes, impacting the release of radionuclides from the repository.

VI-2.2. The far-field model

In the first step, a far-field model was developed using the conceptual model provided by UKR, with a discrete horizontal and vertical fracture embedded into a porous matrix. Unlike the models developed by UKR and LIT, constant head boundary conditions were specified on the sides of the model domain. In the base case analysis, a constant concentration boundary condition was imposed at the repository location. Sensitivity analyses were performed with respect to the head gradient imposed across the model. Moreover, the impact of a horizontal and vertical fracture was evaluated.

In a second iteration, it was assumed that a fracture with variable aperture intersects the disposal area, reaching a well. Dissolved radionuclides are transported in the flow domain by advection and hydrodynamic dispersion. The dissolved concentrations are reduced by sorption in the rock matrix and radioactive decay. The fracture influence on the hydraulic head distribution in the computational domain has been studied.

VI-2.3. Coupled TH effects

The influence of coupled TH effects on the temperature distribution in the repository was compared to the results obtained for the thermal approach.

VI-3. RESULTS AND DISCUSSION

VI-3.1. The near-field model

In the first round of calculations, the release of radionuclides from the repository was assessed taking into account two hydrogeological cases: flow through porous medium and flow through an horizontal fracture crossing the unaltered granite layer. The influence of geosphere conceptualization (porous media vs. fractured media) was assessed through analysis of the release rates out of the repository and the cumulative contaminant quantities released.

It has been shown that the contaminant release rates for the fractured medium are higher than for the porous medium. For all the cases considered, the activities released from the repository for the fission products and for some actinides (Pu-244, Cm-247) show no difference, given the large simulation time ($T = 1.1 \cdot 10^7$ years) compared to their half-lives. For the rest of the nuclides, the released activities and release rates are proportional to the groundwater flow. The mobile inventory in the container at the end of the scenario depends linearly on groundwater flux, for low soluble radionuclides contained in the fuel and cladding, while the rest are insensitive to that parameter. The trend is maintained also for the radionuclides flown out from the buffer. In all the situations considered, at the end of the scenario, all radionuclides in the container were mobilized, due to completion of the fuel and cladding dissolution. Contaminants are either contained in the buffer (especially highly sorbed actinides and cladding activation products), or already left the near-field.

In the iteration of the far-field modelling, the influence of the fracture aperture crossing the disposal field was evaluated. As a consequence of the variation of the aperture of the fracture intersecting the disposal boreholes, the flow of water in the EDZ of the disposal boreholes changes and that impacts the release of radionuclides from the repository.

An increase in the fracture aperture by a factor of ten increases slightly the release out of the repository of well-sorbed nuclides, but has almost no effect on weakly-sorbed nuclides.

The effects on the releases from the near-field of two types of boundary conditions at the interface between buffer and the host-rock were investigated: ‘zero concentration’ and ‘zero flux’. The first condition maximizes the mass transfer out of the facility, but it does not accurately calculate the concentrations at/near the boundary. The second boundary condition maximizes the concentration at the boundary, at the expense of accuracy in calculating the flux through the boundary.

Release from the near-field of Iodine is greatly influenced by the boundary conditions imposed on the buffer-rock frontier and by a lesser extent by the flow conditions. The ‘zero flux’ boundary condition gives much higher concentrations at the buffer-rock interface, which are delayed (their maxima occur after the matrix dissolution time) and almost constant. The influence of the fracture aperture (the water flux in the disposal borehole) is negligible. The ‘zero concentration’ condition gives rise to much earlier pulse-shaped releases, and their maxima are between seven to eight orders in magnitude lower (depending on the fracture aperture) compared to the results obtained for the previous boundary condition. The breakthrough curves in the well are also greatly influenced by the choice of the boundary conditions in the source term. The ‘zero concentrations’ breakthrough curves are faster and have much lower maxima then the ‘zero flux’ outputs. The flow velocity in the domain has a smaller influence on the breakthrough curves compared to the type of the boundary condition imposed at the buffer-rock interface.

VI-3.2. The far-field model

The first geosphere model implies flow in a porous layered domain (with or without horizontal fracture) subjected to a horizontal gradient. From conservative considerations, it was supposed that the head in both the fractured and monolithic granites exceeds the head in the sedimentary covers. The aim of our model is to simulate the possibilities of migration of the leaked plume from the repository into the fractured granites.

Sensitivity analyses were performed with respect to the head gradient imposed across the model. Moreover, the impact of a horizontal and vertical fracture was evaluated. Hydraulic heads and concentration distributions were calculated for the considered variants.

The second iteration in the far-field modelling implied consideration of a fracture that reaches the surface in a well. Boundary conditions were changed, and the influence of a well and a river has been assessed.

The hydraulic spectrum in the flow domain is affected by the fracture geometry. For each fracture aperture (and its associated release rate from the repository), four aspects have been examined: a) the consequences on the hydraulic head distribution, b) the effect of the hydraulic head differences between the well and a river located at the right upper corner of the flow domain, c) the effect of the boundary condition at the interface between the buffer and the rock, and d) the influence of the conceptualization of the sorption in the rock matrix on contaminant transport. For the first three issues, 2D flow and transport calculations were performed using FEFLOW and PORFLOW codes. The fourth study was conducted using the 1D transport code CHETMAD.

The simulations of the water flow show that, due to the conductivity contrast, the main flow is concentrated into the sedimentary cover and only a small part of the water penetrates into the basement. A thin fracture (0.1 mm) does not modify the general flow characteristics, while a large fracture (1 mm) does: the fracture becomes a preferential flow path that discharges all the collected water into the well (independent of the head difference between the well and the river).

Two radionuclides have been chosen to illustrate the contaminant transport: long-lived, weakly sorbing and very soluble I-129, and strongly sorbing Se-79. For a thin fracture, the transport of iodine shows two stages: initially the I-129 is directed along the fracture and (after 20,000 years) the transport is in accordance with the main hydraulic spectrum. I-129 discharges into the river, and the breakthrough curve has a unimodal shape when both tributaries have the same level. When the drawdown in the well exceeds the river level, the breakthrough curve has a bimodal shape. The first maximum is due to the transport through the fracture, while the second maximum is due to the transport according to the regional hydraulic gradient. The breakthrough curve of Se-79 has a unimodal shape. For the large fracture case, all the contaminant is drained by the fracture, as it is suggested by the head distribution, irrespective of the head differences between the well and the river. The effect of the drawdown in the well consists in an increase of the relative peak value. The breakthrough curves shapes are unimodal.

The release rates from the geosphere, and the dissolved concentrations transported with the groundwater are influenced by the fracture aperture, the penetration depth and the sorption properties of the nuclides into the rock matrix. The release of weakly-sorbing radionuclides increases in the case of limited storage capacity of the small fractures walls. At larger fracture openings, there is almost no influence of the storage capacity of the rock on dissolved concentration. At more significant sorption and small fractures, limitation of the matrix diffusion brings forth an increase of the maximum released concentration and flux. The effect is significantly less important when the fracture is wider.

VI-3.3. Coupled TH Effects

As a first step to assessing coupled TH effects, conductive heat transfer was calculated using a rather detailed model of the repository system. The analysis, which did not include coupled effects, was performed using the general-purpose finite element code ANSYS. Heat output from spent nuclear fuel was specified as a time-dependent function, and temperatures throughout the model domain were calculated. Further refinements took into account coupled thermo-hydraulic processes. The maximum temperatures in the repository are higher compared to the thermal analysis, and they occur earlier. In order to increase the capabilities regarding modelling of coupled THM processes, Romania benefited of excellent training at Cardiff University, financed by IAEA.

VI-4. CONCLUSIONS

Studies show that uncertainties in predicting the fate of a disposal system arise from a diversity of factors, from site selection, system conceptualization to modelling approach. It is necessary to conduct careful site investigations in order to avoid preferential pathways for contaminants. In-depth knowledge of the site is needed since even thin fractures can affect the performance of the disposal system. The modelling approach has been proved to be a sensitive matter with respect to system performance. Choice of the boundary conditions influences greatly the response of the system, and considering the TH couplings in the repository point to elevated temperatures in the short term, which can affect the performance of the engineered barriers.

Reference to Annex VI

[1] CHIANG, W. H., KINZELBACH, W., 3D Groundwater Modelling with PMWIN, Springer Verlag, Heidelberg, Germany (2001).

[2] MCDONALD, M.C., HARBAUGH, A.W., MODFLOW – A Modular Three-Dimensional Finite Difference Ground-water Flow Model, USGS Open-file report 83-875, Chapter A1, U. S. Geological Survey, Reston, VA (1988).

[3] ZHENG, C., MT3D – A Modular Three-Dimensional Transport Model for Simulation of Advection, Dispersion and Chemical Reaction of Contaminants in Groundwater Systems. – S.S. Papadopulos & Associates, Inc., Rockville, Maryland, prepared for the US EPA Robert S. Kerr Environmental Research Laboratory, Ada, Oklahoma (1990).

[4] ZHENG, C., WANG, P.P., MT3DMS – A Modular Three-Dimensional Multispecies Transport Model for Simulation of Advection, Dispersion and Chemical Reactions of Contaminants in Groundwater Systems, Documentation and user’s guide, Departments of Geology and Mathematics, University of Alabama, Alabama (1998).

Annex VII

UKRAINE COUNTRY REPORT

VII-1. PROJECT OBJECTIVES

The objectives of the Research Contract UKR 13374: “Forecast of radionuclides migration from geological repository at early stages of siting geological repository (as applied to granitoid formations of Korostensky pluton and Chernobyl exclusion zone, Ukraine)” were to:

- Reform radionuclide transport simulation in support of a site suitability analysis for a geological repository within the Chernobyl exclusion zone and adjacent territories;
- Determinate of additional data for model updating, assessment of granite formations’ suitability and identification of hydrogeological factors influencing to the repository safety; and
- Study advanced international experience of applying of numerical simulation in support of site characterization and safety assessment of geological disposal.

VII-2. APPROACH AND SCOPE OF WORK

VII-2.1. Conceptual models, concepts, and principal processes

A deep geological repository (DGR) and its far-field zone were represented by a 2D radial section around the modelled repository. The approach of space-distributed continuous flow and transport parameters for model representation (an equivalent porous medium model), and the finite-difference approach for space discretization were used. The principal flow and transport concept, on which the model is based, is shown on Fig. VII-1. Modelling of radionuclide migration in the geological medium is based on numerical solution of corresponding 2D initial-boundary problems for systems of partial differential equations describing processes of steady groundwater flow (filtration) and unsteady migration of radionuclides in the geological medium at their outflow from a DGR. The model was developed using the 3D Processing Modflow (ver.5.3) hydrogeological modelling system [1]. The system is based on the MODFLOW code for groundwater flow [2], and MT3DMs code for contaminant transport [3, 4].

VII-2.2. Numerical model, boundary conditions, and parameters

The model for the prospective Veresnia site (far-field of DGR) has been developed based on the available data assessments obtained during the previous research for the site. These data include the topology (depths) of the main geological strata, assessed hydraulic conductivity and porosity of the deposits, and groundwater heads observed in the aquifers of active water exchange zones (sedimentary cover and upper zone of fractured granites).

The 1.5 km deep and 5 km long model domain contains 9 layers (Fig. VII-2) each layer being discretized into 100 grid blocks (50 m in length and depth; variable vertical thickness). No-flow boundaries are imposed on the vertical and bottom boundaries; a constant infiltration rate of 100 mm/yr is imposed at the top boundary; a constant head boundary is applied at the upper-right corner, representing a river; a drinking water well in the upper aquifer is simulated with a constant head boundary conditions; in the transport simulations, particles were released and constant relative concentrations were specified on the left boundary at a depth of 800–1000 m, which represents the repository.

Steady-state, saturated groundwater flow was simulated for different conditions in the well, different hydraulic conductivities in the model layers (Table VII-1) and separate blocks (the fracture zone simulation), and for different assumptions about the intensity and duration of the radionuclide release from the near field of the repository.

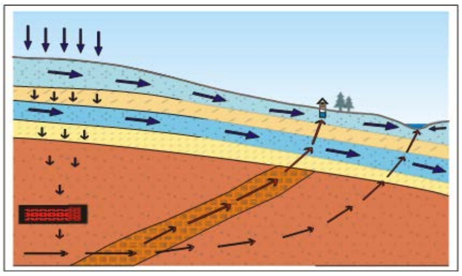


FIG. VII-1. Groundwater flow-transport conceptual model of Veresnia site.

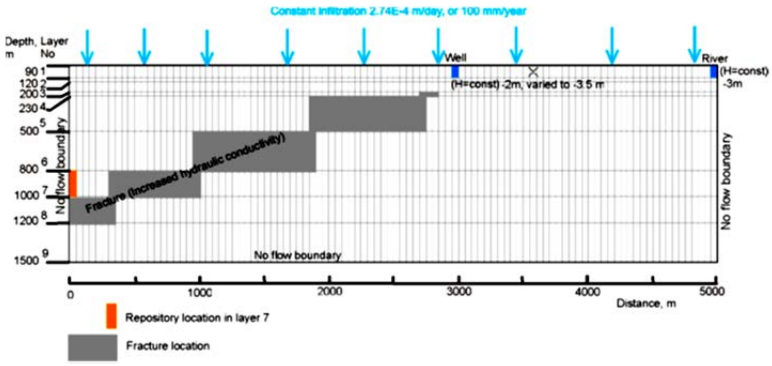


FIG. VII-2. Numerical model and its boundary conditions.

TABLE VII-1. TWO SIMULATION SETS FOR LAYERS HYDRAULIC CONDUCTIVITY

Layer No	Depth [m] (top-bottom)	K_L sets [m/s]		Porosity [-]	Description
		Common	Realistic		
1	0-90	5.0E-4	5.8E-05	0.15	Quaternary + Paleogene aquifer
2	90-120	2.0E-7	2.3E-07	0.01	Confining layer (Paleogene marls)
3	120-200	5.0E-4	1.2E-05	0.1	Cretaceous + Jurassic aquifer
4	200-230	1.0E-7	5.8E-08	0.01	Confining layer (Jurassic clays + weathering bedrock)
5	230-500	5.0E-6	5.8E-07	0.005	Upper fractured zone of bedrock
6	500-800	5.0E-8	1.2E-08	0.002	Monolithic crystalline bedrock
7	800-1000	5.0E-8	5.8E-09	0.002	Monolithic crystalline bedrock, geological repository location
8	1000-1200	5.0E-8	5.8E-09	0.002	Monolithic crystalline bedrock
9	1200-1500	5.0E-8	5.8E-09	0.002	Monolithic crystalline bedrock, lower boundary layer

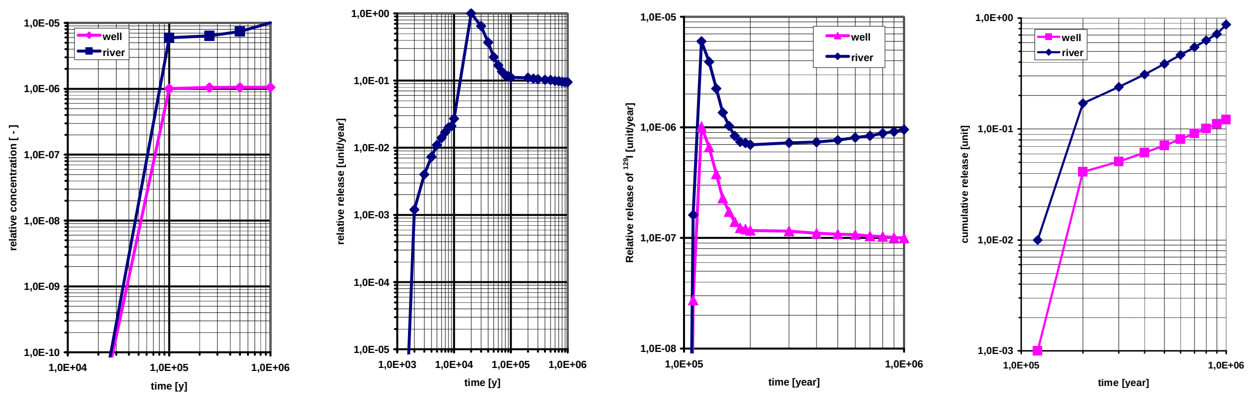
The information on parameters, assumptions, and scenarios describing the DGR near-field zone used by UKR, are specified described in “Ukrainian case specification” (see Annex I).

VII-2.3. Simulation task

All the simulation tasks are concerned with the influence of different model parameter changes on the intensity of groundwater flow and transport of radionuclides from the repository to the discharge zones (well and boundary river). These influences were characterized by contaminant travel time (t_t) and relative contaminant concentration reached at discharge zone locations: the river (RC_r) and the well (RC_w). The simulation tasks are:

- Task 1: study of the effects of hydraulic conditions (heads in the well and layers’ conductivity) in upper aquifers on flow through granite;
- Task 2: study of the influence of a fracture zone;
- Task 3: study of the impact of various release assumptions (release duration, contaminant relative concentration in the source, repository position) on far-field radionuclide transport;
- Task 4: study of the influence of geosphere sorption properties on far-field radionuclide transport.

The near-field release was not calculated by UKR. For calculations of ^{129}I release and cumulative release curves at the well and river boundaries (and for related radiological assessments), the results of the near-field release calculations performed by LIT and ROM teams are used. The implementation procedure of the near-field release results into the far-field model shows on the Fig. VII-3.



(a) RC(t): relative concentration at the discharge points

(b) NR(t): normalized near-field release

(c) NRC(t) normalized release at the discharge points

(d) NCRC(t) normalized cumulative release at the discharge points

FIG. VII-3. Procedure of implementation of the near field release results into the far-field model.

The following *additional research tasks* have been carried out:

- Assessment of equilibrium uranium concentration for the expected hydrochemical conditions of the Veresnia site;
- Mass-balance calculations;
- Preliminary study of sorption effects in sediments and weathering crusts.

VII-3. RESULTS

VII-3.1. Simulation results

VII-3.1.1. Task 1: study of the effects of hydraulic conditions in upper aquifers on flow through granite

Effects caused by the different values of hydraulic heads in the well: Increase of conductivity in the upper layers in the presence of a well or river leads to faster drainage of the upper layers and decrease of the water exchange rate in the deeper layers. As a result, the travel time for the high-conductivity case (common or “pessimistic” set of K_L) in the upper layers is significantly longer as compared with the case when the conductivity is lower (realistic set of K_L). This somewhat surprising result is likely caused by the flow velocity distribution over the vertical model section, which is governed by the hydraulic conductivity distribution and the given boundary conditions.

Effects caused by different conductivity of the first aquifer: The first aquifer’s conductivity exerts significant influence on travel time (i.e. on the assessed repository safety). Increased conductivity of the first aquifer (set at the same conductivity as that of the other layers) results in a significantly longer travel time of the contaminant from the repository to the discharge point (river or well) and a lower final concentration at the discharge point.

Effects caused by different conductivity of the first confining layer: Lower conductivity of this layer leads to longer travel time and lower concentration in the discharge point.

In summary, the *study of the effects of hydraulic conditions in the upper aquifers on flow through granite* has shown that for different assumptions about the well drawdown and hydraulic conductivity of the first aquifer and first confining bed, the assessment rages by:

- One order of magnitude for the travel time;
- Two orders of magnitude for relative contaminant concentrations in the river; and
- Four orders of magnitude for relative contaminant concentrations in the well.

VII-3.1.2. Task 2: study of the influence of fractured zone

The results shown in Fig. VII-4 show a relatively weak sensitivity of the chosen model travel time and relative concentration on increasing hydraulic conductivity in the fracture. This may be explained by possible downward (infiltration) flow of clean water which diverts the contaminant flow in the near field zone of the repository.

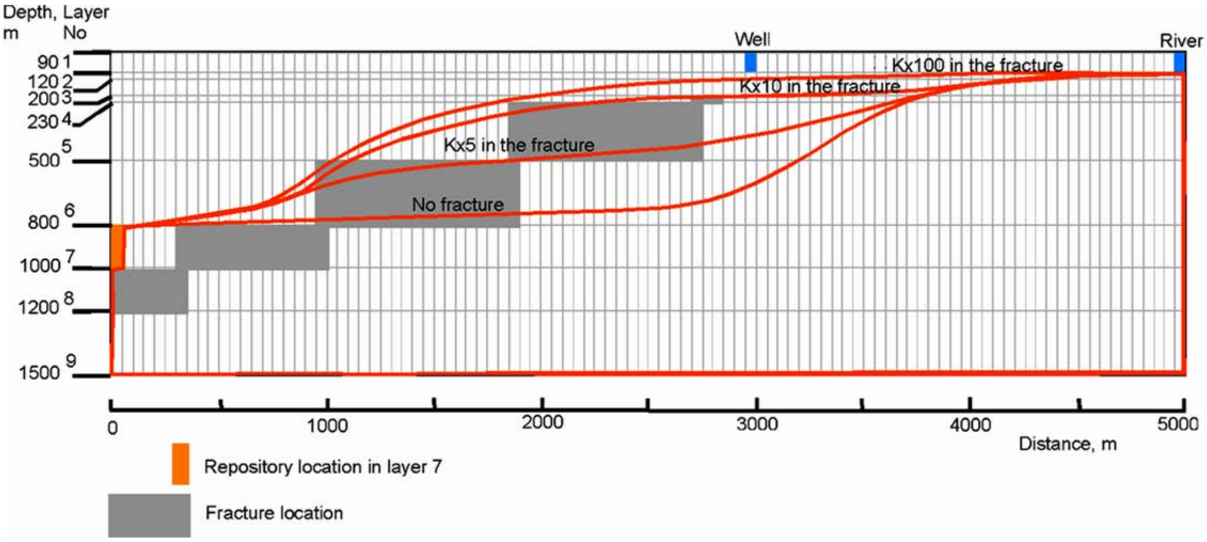


FIG. VII-4. Influence of the fracture (with different factors of increased hydraulic conductivity) on contamination plume spreading. Plume boundaries correspond to a relative concentration $RC/RC_0=10^{-6}$ after 10^6 years.

VII-3.1.3. Task 3: study of the impact of various release assumptions on far-field radionuclides transport

Duration of radionuclide release: After radionuclides are released from the repository (Fig. VI-5), dissolution and advection is dominated by incoming clean water. It causes relatively fast plume displacement and its dispersion. The release duration and time frame is directly related to the overall contaminant balance and concentration variation at the compliance boundaries (river and well).

Source relative concentration: For the given model, the contaminant travel time is independent of the source concentration, and relative concentrations in the discharge points are proportional to the source concentration.

Displacing the repository location: Moving the repository closer to the river or other discharge points that have a smaller vertical flow component (and consequently, a higher horizontal flow component directed to the discharge point) leads to significantly shorter travel times and to higher relative concentrations at the discharge points. Thus, the position of the repository in the downward-flow (watershed) region is essential.

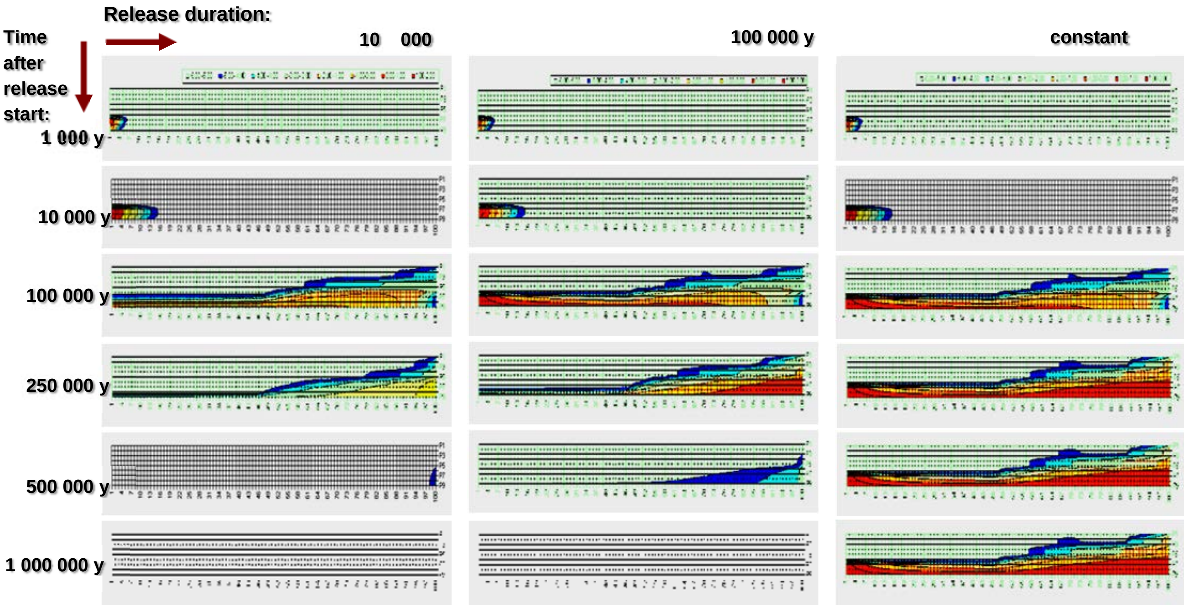


FIG. VII-5. Contaminant plume distribution boundaries for the different release durations.

VII-3.1.4. Task 4: study of the influence of crystalline sorption properties on far-field radionuclides transport

The dimensions of the contaminant plume (see Fig. VII-6) strongly depend on the $K_{d.}$ value. Only non-sorbing radionuclides (for example, ^{36}Cl and ^{129}I) may reach the discharge boundary (river) for the given conceptual model.

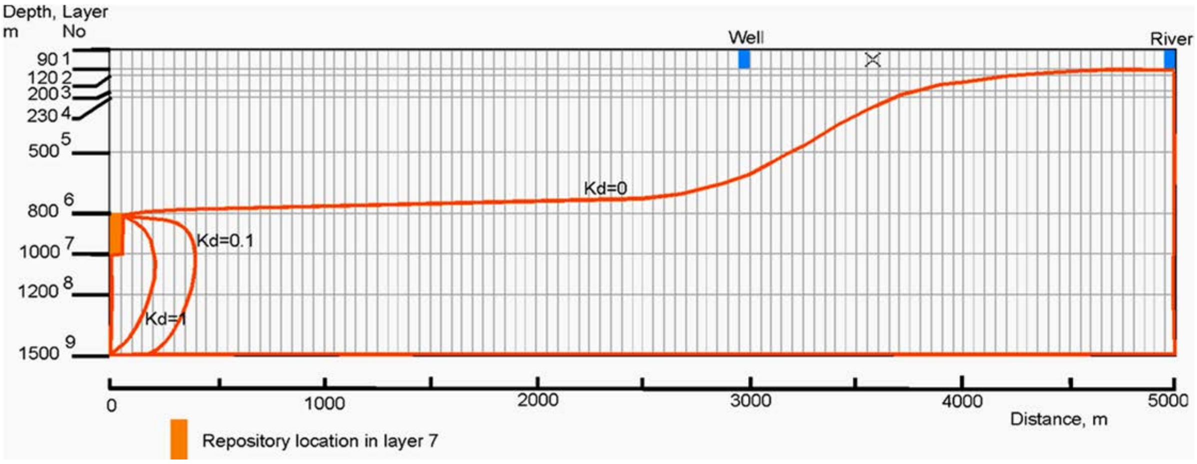


FIG. VII-6. Contaminant plume distribution boundaries for relative concentration $RC/RC_0=10^{-6}$ after 10^6 years at different K_d (L/kg) values.

VII-3.2. Preliminary radiological assessment

The dose range (10^{-6} – 10^{-1} Sv/y) calculated on the basis of the LIT and ROM near field release scenario and UKR normalized breakthrough curves (Fig. VII-7) strongly depends on the assumptions about the release scenario and model parameters (groundwater levels in the river and well, set of K_L). For this reason, the currently obtained results of radionuclide transport modelling still cannot be used directly for geological repository safety assessments.

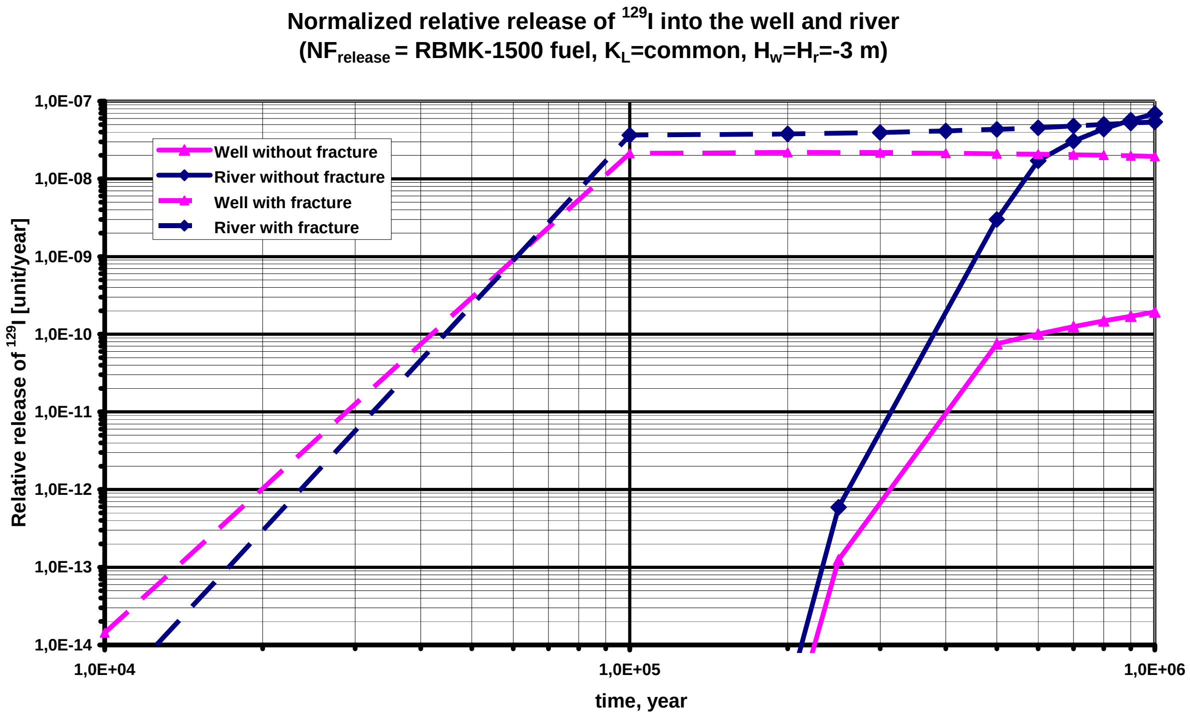


FIG. VII-7. Relative normalized (to the initial inventory and to the container failure time) release at the well and the river (equivalent porous medium model with and without a fracture zone).

VII-3.3. Additional results

Simulation of Uranium dissolution: The modelling results have shown that for the expected hydro chemical conditions at the repository location depth within the Veresnia site (temperature: 10-20°C, pH < 7,5 and reducing conditions) the equilibrium uranium concentrations in the groundwater should range between 10^{-8} and 10^{-7} mol/l. The maximum UO_2 dissolution occurs under pH from 8 to 10.5 ($>1\cdot10^{-5}$ mol/l).

Mass-balance calculations show that matrix dissolution rates range from 10^{-11} to 10^{-10} y^{-1} for reasonable combinations of U solubility and groundwater flux. This means that under likely hydraulic and hydro chemical conditions at the repository depth, radionuclides will be released slowly and for a very long time, approaching a steady-state contaminant source regime.

Increased waste matrix solubility to values used for modelling of the contaminant source (10^{-7} – 10^{-4} y^{-1}), and using realistic groundwater flux values, are possible if oxidizing conditions are reached at the repository level, and/or the pH of the groundwater is in the range between 8 and 10.

Reasonable matrix dissolution rate should be determined taking into account realistic local hydro chemical conditions, fluxes and solution/waste ratios at the depth of the repository. These data should be obtained based on field studies.

Sorption effects in sediments and weathered crusts: The sedimentary rocks of the Veresnia site are mainly (80%) composed of clays and loams characterized, which exhibit rather high K_d values for the principal radiologically significant nuclides (besides iodine). These sediments (as well as the weathered crust) have a significant sorption potential. Consequently, their barrier role should be accounted for in geological repository safety assessments.

VII-4. MODEL SENSITIVITY AND UNCERTAINTIES

Influence of primary model settings and assumptions: Assumptions about (a) the primary far-field hydrogeological model related to the geometry and main flow pattern over the section, and (b) the initial near field conditions have the strongest influence on the compliance measures. In particular, the release curves strongly depend on recharge and discharge locations and intensity, on boundary conditions (specifically the presence of a no-flow boundary along the right model side), and on the release scenario. These model features thus need to be properly justified. The geometry of the cross section, its depth structure, and the repository location (800-1000 m deep in the central portion of the watershed) were selected based on preliminary analyses of the general geological and hydrogeological structure of the proposed Veresnia site. Changes of the release scenarios also have a strong influence on the compliance measures. For this reason, the most conservative and easy to simulate (and recalculate) case of idealized “constant initial relative concentration” release source was considered as the base case.

Influence of flow and transport parameters: Besides the primary model assumptions (such as recharge and discharge pattern and intensity), the hydraulic parameters of the top water exchange zone (layer 1) such as conductivity and drawdown in the river and well strongly influence the compliance measures. The surprising result is that higher drainage activity and hydraulic conductivity in the upper layer may provide a “safer” situation in the deeper (repository horizon) layers, because it intercepts the most part of the downward groundwater flow of the watershed at early stages of its formation. Under these conditions, the top and most active water-bearing layers (Quaternary, Eocene) may have a key impact on the water exchange intensity in the deep (repository) zone.

The most influencing transport parameters include the distribution coefficient of the host crystalline rock around the repository and along the main transport pathway from the repository to the discharge point. This parameter depends on both rock and contaminant (radionuclide) properties. Non-sorbing radionuclides (for example, ^{36}Cl and ^{129}I) lead to conservative estimates of transport times.

Model parameter uncertainties: The main reason for parametric uncertainties is insufficiency or absence of direct field and experimental investigations for the modelled Veresnia site. However, modelling may cover the reasonably accepted range for these parameter uncertainties taken from the literature, hydrogeological handbooks for the rocks and geological beds of the studied area, etc. The parameter ranges and their influence on the results is a subject of model sensitivity analysis, as described above. Among the principal parameter uncertainties, the following should be mentioned:

- Groundwater hydraulic head distribution;
- Conductivity and porosity for different model layers;
- Matrix and fracture K_d values under existing hydro chemical conditions.

The uncertainty of the boundary hydraulic heads in the upper model layer of the simulated Veresnia site (Quaternary and Paleogene aquifers) ranges from 1 to 90 m. However, for most of the area the levels are determined with accuracy range between 1 and 10 m. The head uncertainty will be decreased in the course of further site characterization (drilling and observation in boreholes and shallow wells). In the model section this uncertainty is partly addressed by calculating initial groundwater head distributions accounting for areal groundwater recharge taken as the basic parameter, and considering drawdowns in the discharge points. The groundwater head distribution in the deep crystalline base is mostly unknown, and only a hypothesis is accepted about the downward flow pattern within the watershed area considered for the repository location.

The uncertainties of conductivity taken in the model generally may be assessed within one to two orders of magnitude. The model values are taken according to available literature data for the site conditions. The influence of these uncertainties has been assessed in the model sensitivity analysis described above.

The uncertainty of K_d is relatively small for known radionuclides and host rocks. However, this information is not always known, and given the strong impact of K_d on transport simulation results, its value and uncertainty must be carefully determined.

Model simplification uncertainties: Concerning the described model, the following conceptual model uncertainties must be mentioned:

- Neglecting the dispersion and/or sorption;
- No-flow boundary conditions for bottom and right model boundaries; and
- A single fracture zone instead of a network of discrete fractures.

The main uncertainties related to the absence or insufficiency of initial data corresponding to realistic conditions of the repository, were replaced, where feasible, by conservative assumptions. For example, to study the most conservative case for the concentration values along the main contaminant pathway, the dispersion coefficient was taken to be zero in the deterministic transport simulation series, and pure advective transport was considered, using the MODFLOW and PMPath codes. This simplification was accepted given the general physical nature of dispersion, which summarizes a number of physical mechanisms (splitting of elementary flows, pore tortuosity and open space variations, anisotropy and scale dependence, etc.), as opposed to the formal, mathematical nature of the dispersion tensor.

Accepting the simplified non-permeable horizontal model boundary at the right end of the model section requires that all the incoming groundwater discharges at the river. In reality, a significant part of the flow may continue to travel in the horizontal direction at depth, passing under the river and wells, and only a potentially small portion will come upward to the discharge point. If we suppose the model area to be extended in the horizontal plane and account for a lower drainage ability of small rivers of the Veresnia site, then the contamination front will not reach the modelled small river, but will proceed deeper to Pripyat or even Dnieper in the scale of Dnieper-Donets depression region.

The simplification uncertainties are inevitable. However, in our case we tried to satisfy the principle of conservatism of the expected result assessment, and gradual decrease of conservatism with increasing detail of the “stage-by-stage” object study. For example, the single ascending fracture zone (instead of fracture network) was taken, which directly connects the repository to the discharge well, and different conductivity series in a wide range of values have been simulated to assess the range of its possible influence.

The model *oversimplifications* such as constant head and no flow boundaries, constant source concentrations, pure advection model scenarios, highly increased conductivity in the fracture (5x, 10x, 100x), etc. should also satisfy the conservative approximations principle (taking the “reasonable-worst” case as the base case), and on the other hand, allow obtaining “upper and lower limit” assessments for the expected results (advection travel time, etc.) giving in such a way the assessment framework for further modelling stages (based on more refined observation and parametric data).

The most common reason of acceptance of the oversimplification (highly conservative) model conditions is absence of detailed data of hydraulic parameters and the detailed concept of the repository.

The *model scenario uncertainties* include:

- Start and duration of release; and
- Possible increase of release intensity with time.

These uncertainties are overcome mainly using the recalculation procedures with taking as the base simulation case a constant initial relative concentration in the source, and balance assessment of local flow rates in the source and discharge model blocks.

The apparent contradictions between some results of (advection) travel time and final concentration assessments are explained by different scope and purposes of physical models of pure advection and convection-dispersion transport (and their corresponding codes PMPATH and MT3DMS). However, both models give good comparison assessments and greatly improve our representation about the main directions and comparative time scales of the transport process from the repository to the far-field zone.

VII-5. CONCLUSION

The main indirect safety characteristics of the repository, such as the predicted contaminant concentrations and travel times to the discharge boundaries (wells, rivers), mostly depend on the location and drainage ability of the rivers and wells, and the hydraulic conductivity and sorption capacity of water-bearing deposits. Furthermore, changes in hydraulic conductivity affect the shallow and deep convection pattern, leading to significant changes in predicted transport behaviour as a result of uncertainty in the spatial distribution of hydraulic conductivity. Changes in fracture hydraulic conductivity and sorption coefficient have the expected effect on radionuclide concentrations in the river or well.

The presence of distributed shallow (low-drainage) discharge wells or small rivers — given the general characteristics of the watershed with downward infiltration and well-developed covering deposits — is not an unfavourable factor for repository safety. Under such conditions, infiltration is mainly intercepted in the upper layer, and the deeper geological medium remains the intact zone of slow groundwater flow and slow contaminant transport.

In addition to large variations in the calculated travel times as a result of uncertainty and variability in the hydrogeological input parameters for the geosphere, predicted radionuclide fluxes as well as peak and cumulative concentrations further depend on the chosen release scenario, resulting in many orders-of-magnitude differences in the predicted dose.

Main uncertainties of the results reflect the current situation and the level of development of the radioactive waste disposal programme in the Ukraine. This level is characterized by:

- Absence of clear concepts of waste disposal with determination of the repository design and type of container;
- Very restricted data on the waste inventory and possible radioactive release scenarios;
- Restricted data about geological and hydrogeological characteristics of the prospective sites.

For this reasons, the results of radionuclide transport modelling obtained in the UKR 13374 project cannot be directly used for geological repository safety justification at the Veresnia site. They may strongly depend on the initial assumptions. The mechanical and thermal processes occurring in the geological repository system and exerting significant influence on the repository safety have not been considered in the framework of this project. The radionuclide concentration assessments are based on the near field zone concept and the evolution scenarios (start of radionuclides release), which may not be consistent with the repository concept that will be developed for the Ukraine.

Nevertheless, the investigations performed as part of this project allowed identifying several factors that may increase the repository safety and may be used in the future for the development of the siting criteria. They are:

- High conductivity of the upper aquifer and lower conductivity of the confining layers;
- The high vertical gradient of layers conductivity above the repository;
- Placement of the repository at a location where vertical downward movement of groundwater is dominant;
- Presence of sedimentary cover and granite weathering crust;
- Presence of sulfide minerals in the rock fractures at sites of upward groundwater flow to the discharge zones.

The uncertainty of the main modelling results of the UKR 13374 project shows the importance and necessity of conducting detailed field investigations of the potential sites, and the development of a national concept for a geological repository. Besides this, knowledge about processes of nuclide migration, retardation and immobilization can be essentially increased by the balance calculations taking into account existing hydraulic, hydro chemical and geochemical conditions.

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