Title
The use of numerical models in support of site characterization and performance assessment studies for geological repositories

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of geologic repositories

An IAEA Coordinated Research Programme

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Summary

The paper is describing work being developed in the frame of a 5-year IAEA Coordinated Research Programme (CRP) started in late 2005. Participants gained knowledge of modelling methodologies and experience in the development and use of rather sophisticated simulation tools in support of site characterization and performance assessment calculations.

These goals were achieved by a coordinated effort, in which the advantages and limitations of numerical models are examined and demonstrated through a comparative analysis of simplified, illustrative test cases. This knowledge and experience should help them address these issues in their own country's nuclear waste program.

Coordination efforts during the first three years of the project aimed at enabling this transfer of expertise and maximizing the learning experience of the participants as a group. This was accomplished by identifying common interests of the participants (i.e., process modelling and Total System Performance Assessment methodology), and by defining complementary tasks that are solved by the members of the cases. Synthesis of all available results by comparative assessments is planned in the coming months. The project will be completed end of 2010. This paper is summarizing activities up to November 2009.

Introduction

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*" is to transfer modelling expertise and numerical simulation technology to countries requesting them for their national nuclear waste management programs.

Numerical modelling is a key component of any nuclear waste isolation program. Simulation and optimization technologies are used to (1) improve the understanding of complex coupled processes in the subsurface, (2) integrate available characterization data (geologic features as well as the hydrologic, thermal, chemical, biological, and mechanical behaviour of the repository system) into a comprehensive conceptual model, (3) design laboratory and field experiments and analyze the resulting test data, (4) reproduce the observed state of the natural system, and (5) predict the performance of the proposed repository system over extended time periods, using sometimes scare site-specific data.

Participation

The five-year CRPs started on October 1, 2005 after evaluation of the initial research proposals from potential participants in view of practical integration of interests, expertise and tools (e.g. code application and development, processes). IAEA has awarded for this CRP five Research Contracts (work programme linked to limited funding) 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)*; Radioenvironmental Centre of National Academy of Science of Ukraine, Department of Hydrogeological Modelling

In addition, the following two Research Agreements (financial support to attend coordination meetings only) were awarded:

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

The following Member States are supporting and guiding this CRP as scientific coordinators (financial support to organise and guide coordination meetings):

- *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 (USA)*; Lawrence Berkeley National Laboratory (LBNL), Earth Sciences Division

Research activities are coordinated by IAEA and supporting Member States at Research Coordination Meetings (RCMs) taking place each 18 months. Progress is monitored through review of deliverables. Contract renewal is contingent on proposal quality and performance. When possible, CRP activities may benefit from the participant's attendance of various training courses on similar subjects, sponsored by IAEA through the Technical Coordination (TC) Programme.

Phase 1, which covers the period up to September 2008, is documented in various progress and synthesis reports on which this paper is mainly based. It will also include information on the content and expected outcomes of Phase 2 of the project now running, following discussions that took place in November 2009 at the last coordination meeting.

Coordination Meetings

RCM 1: Beijing, China, September 2006

The first-year progress reports provided insights into the repository systems and simulation approaches considered by each participant. While progress has 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, which was held in Beijing, China, September 11–15, 2006. The discussions resulted in a coordinated effort to focus on a set of common objectives, and cases were developed to be jointly examined by all participants. To better align the project with the overall goals of the CRP, two main topics of common interest were identified, dealing respectively with process modelling and Total System Performance Assessment (TSPA) methodology. The objectives and general approaches for the two groups are briefly described below.

Group A: Process Modelling

The main objectives were: a) to develop and use numerical process model for a generic repository in a crystalline host rock to support site characterization and performance assessment, b) to perform sensitivity analyses to identify key parameters, features, and processes, c) to examine uncertainty resulting from differences in conceptual models, scenarios, and supporting data, and d) to provide simulation results to Group B.

The group members were CPR (lead), LIT, ROM, UKR, with support from IND, KOR. The general approach was defined as follows:

- Develop a process model of a generic site based on a description provided by UKR; additional generic data and their uncertainties are provided by CPR based on borehole data from the Beishan site (similar potential host formation);
- Near Field: describe a generic repository system based on the Swedish concept (LIT); identify key radionuclides and source term (ROM);
- Far Field: Develop up to 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 (KOR);
- Perform process model simulations of groundwater flow and radionuclide transport; calculate performance measures at potential compliance boundary; conduct sensitivity analyses;
- Compare simulation results to assess prediction uncertainties;
- Provide distributions of simulation results (source term, radionuclide release rate from engineered barrier system (EBS), radionuclide flux at compliance boundary) to Group B.

Group B: TSPA Methodology

The main objectives were: a) to demonstrate total system performance assessment (TSPA) methodology by developing simplified TSPA models, b) to compare alternative TSPA methodologies (probabilistic assessment using Monte Carlo simulations (CPR); possibilistic assessment using fuzzy logic (BRA)), c) to provide results of impact analysis to Group A.

The group members were BRA (lead) and CPR. The general approach was defined as follows:

- Define components of repository system to be included in simplified TSPA model;
- Develop simplified TSPA model for radionuclide migration analysis;

- Select key parameters and their uncertainty distributions;
- Define performance measure;
- Run TSPA model and compare results;
- Identify key parameters as well as key features, events, and processes (FEPs) affecting repository performance and report to Group A.

RCM 2: Daejon, Korea, May 2008

The second Research Coordination Meeting was held in Daejon, Korea, May 19–23, 2008, hosted at KAERI offices. 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 a Mid-Term Report (August 2007). Communication of results and coordination of research activities within and across the two groups proved to be challenging. To enable successful completion of Phase I of the CRP, new scenarios were defined, and a schedule with milestones and deliverables were provided. Besides individual annual progress reports, both group leaders were asked to provide a synthesis report.

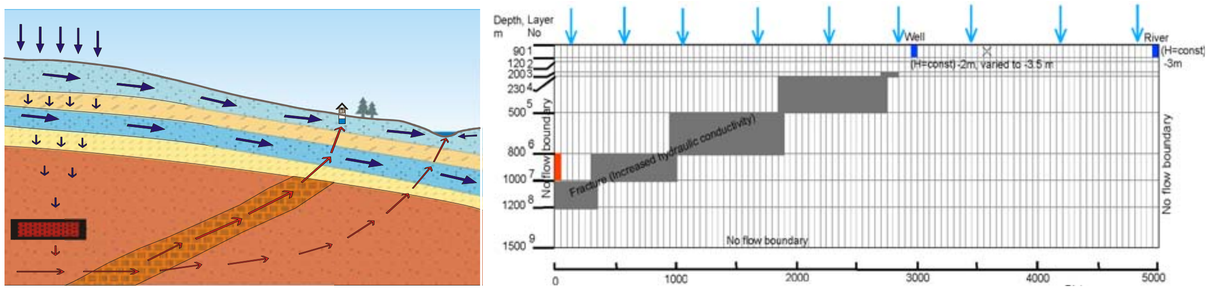
RCM 3: Kaunas, Lithuania, November 2009

The third Research Coordination Meeting was held in Kaunas, Lithuania, November 9–13, 2009. Discussions of research results and pending actions were directly related to the final year of the project and reporting. The work to be performed for the final year was restructured in response to the discontinuation of the contract with BRA; a comparative analysis of probabilistic and possibilistic performance assessment analyses was considered unfeasible in this frame given the results developed during the first three years of the CRP. Based on a summary list of simulation cases, objectives were identified suitable for a comparative analysis. Four comparison studies were proposed. Two studies relate to near-field behaviour and aim at examining a) how the conceptual model and the choice of a computer code affect release curve calculations, and b) how differences in the disposal concept lead to different radionuclide releases from the engineered barrier system. Two comparative studies of far-field simulations examine 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.

Example of preliminary results in phase 1

Ukraine

A regional, two-dimensional flow and transport model was developed, representative of the Ukranian generic site. The conceptual model and the corresponding numerical model are shown in Figure 1. In addition to an equivalent porous medium model (with a layered hydraulic conductivity structure), a variant of the model includes a discrete fracture zone, allowing for a potential fast-flow pathway from the repository to shallow aquifers and the compliance boundary.



(a) (b)

Figure 1. Conceptual and numerical model of Ukrainian site (Shybetskyy et al., 2008, Figures 1 and 2).

Flow and transport simulations were performed using the PMPath code (Chiang and Kinzelbach, 2001), a Windows software package based on the MODFLOW suite of 3D finite-difference flow and transport simulators. A base-case scenario was defined (with radionuclide release from a single defect canister starting 1000 years after waste emplacement), and performance measures (pressures, flow rates, relative concentration flux, and cumulative release curves for ^{129}I and ^{79}Se at specified control points within the model domain) were established for subsequent model comparisons.[1] The flow fields and corresponding advective transport times from the repository to a discharge point (river or well) as well as relative contaminant concentrations were determined for varying well drawdowns, boundary head, sorption coefficients, and hydraulic conductivities. In addition, the impact of the fracture zone (and its conductivity) was analyzed. Examples are shown in Figure 2 (impact of fracture zone) and Figure 3 (relative flux of ^{129}I[2]).

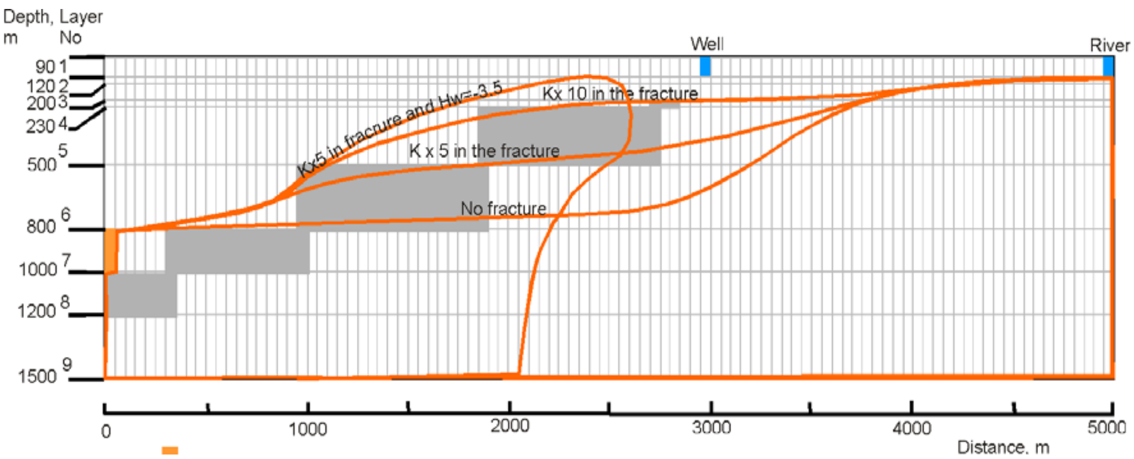
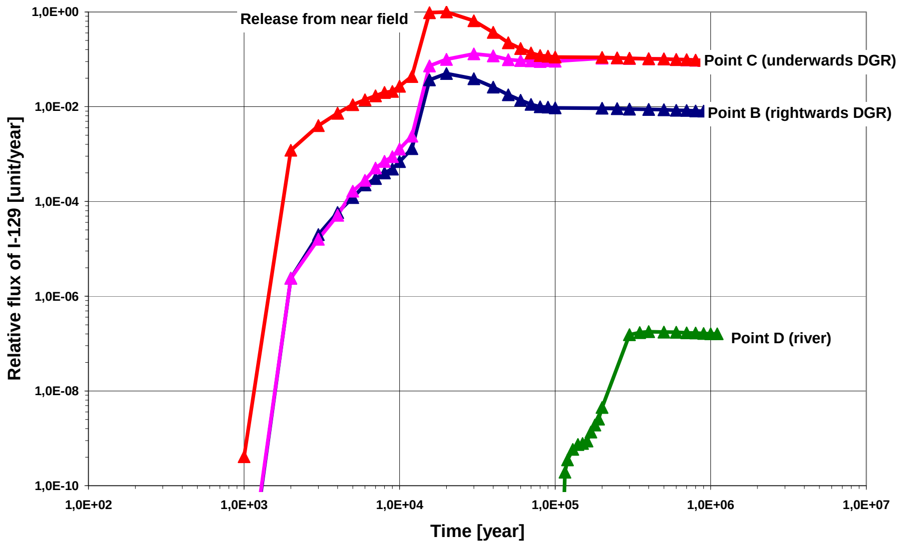


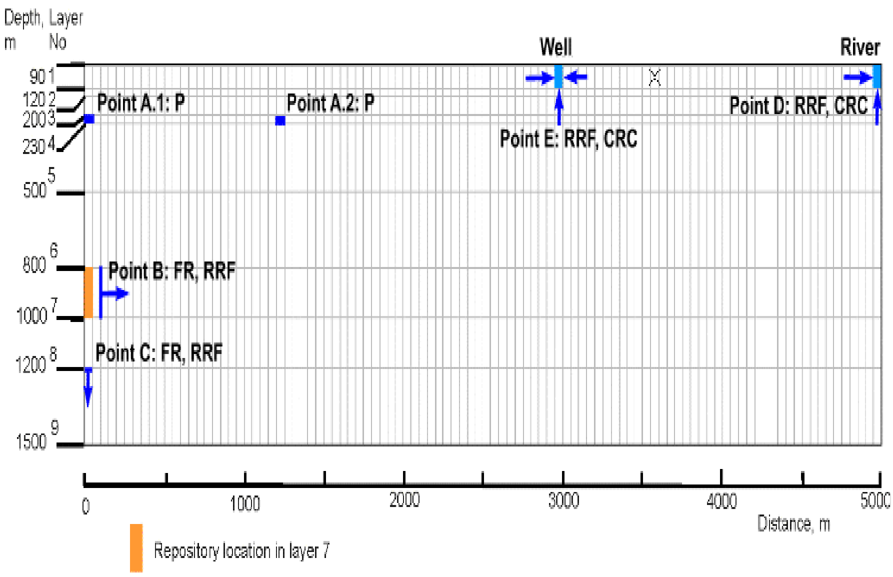
Figure 2. Influence of fracture zone and its hydraulic conductivity on contamination plume migration. Plume boundaries correspond to relative concentration $C/C_0=10^{-6}$ for a simulation time of 10^6 years (Shybetskyy et al., 2008, Figure 7).

[1] Initially, a base-case scenario and performance measures were proposed by the Lithuanian team (Brazauskaitė et al.,2008)

[2] Relative flux of ^{129}I for different points was calculated on the base of LIT relative radionuclide release curves from near field (Brazauskaitė et al.,2008)



(a)



(b)

Figure 3. (a) Relative flux of ^{129}I at different control points as a function of time; (b) location of control points within model domain (Shybetskyy et al., 2008, Figures 8 and 10).

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 affects radionuclide migration, breakthrough times, and relative concentration. 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. 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.

Other contributions

Lithuania focused on near-field modelling and source term determination, based on the Swedish KBS3 concept, which was adapted to Lithuanian conditions. Specifically, deterministic and probabilistic relative radionuclide release curves from the engineered barrier system for ^{129}I and ^{79}Se were calculated. An equivalent porous medium approach was used for the far-field modelling. Flow and transport predictions were made for 1 million years using the TOUGH2 simulator. Sensitivity analyses with respect to hydraulic conductivity, porosity, and sorption coefficient were performed. The impact of coupled thermal-hydrological effects was evaluated by simulating heat- and gas-generating nuclear waste. The AMBER, COMP23, COMPULINK, and TOUGH2 simulators were used for this exercise.

Romania considered the optimization of the repository design for CANDU fuels. The DUST code is used for near-field simulations. Different container degradation models were evaluated, accounting for multiple release mechanisms and related hydrogeological and geochemical parameters. Insights into parameter sensitivities for ^{129}I and ^{79}Se were gained. For the far-field, a conceptual model similar to that used by UKR with an embedded tectonic fault was developed, and flow and transport simulations were performed using the FEFLOW code with relatively high spatial and temporal resolutions. Thermal-hydrological-mechanical coupling issues are also discussed.

China analysed a simplified repository system using probabilistic Monte Carlo simulations by means of the GoldSim system-level modelling tool. A conceptual model (a one-dimensional fracture zone embedded in a porous matrix of low permeability) is implemented into the GoldSim simulator. The sensitivity of the predicted ^{129}I and ^{79}Se concentration in the river and the dose received by a receptor with respect to 15 selected input parameters. A determinist simulation using base-case parameters was also performed.

The Korean research agreement holder KAERI provided a summary report on discrete fracture network (DFN) simulations of the reference site (Kang and Jeong, 2008). The general outline follows the conceptual model described by UKR, but is expanded to 3D. The DFN is an alternative conceptual model to the continuum approaches used by UKR, ROM, and LIT. Groundwater flow path lengths from the repository and travel times are determined, as well as radionuclide release curves from the near and far fields for ^{129}I and ^{79}Se.

Continuation of CRP (Phase 2)

The approach developed in phase 1 has been largely successful. Specifically, Group A employed numerical process models and applied them to a representative repository system. Group members produced complementary results for near-field radionuclide releases and far-field transport. The individual choices of scenarios and model variations allowed the participants to examine country-specific conditions, while at the same time contributing to the overall understanding of the impact of various modelling decisions on prediction results. Group B had the opportunity to discuss and examine alternative TSPA methodologies, the corresponding data needs, the computational requirements, and the interpretation of the sensitivity and uncertainty results. Both groups benefited from each other's accomplishments. Group A results provided the needed input for a TSPA calculation, and the TSPA analyses of Group B, when completed, will help identify key aspects of a modelled repository system that need to be better characterized and further analyzed.

To fully realize the benefits of the approach started in Phase I of the CRP, the analyses need to be partly realigned, expanded, and completed, which would be the overall scope of Phase II. Specifically:

- Group A could expand the modelling cases of the generic site to include one or several of the following:
  - Add scenarios (design concepts, failure scenarios, climate scenarios, etc.)
  - Perform coupled subsystem simulations (canisters, engineered barriers, near field, far field, host rock, overburden, etc.)
  - Perform coupled process simulations (thermal-hydrological-mechanical-geochemical)
  - Examine site characterization, test design, and data integration issues (inverse modelling)
- Group B could complete, update, and refine the TSPA model (probabilistic), including one or several of the following:
  - Include new data and parameter correlations into TSPA analysis
  - Refine model and propagate uncertainty through multiple model components
  - Include mutually exclusive scenarios into TSPA evaluation
  - Perform an impact analysis that clearly identifies key features, events, and processes that significantly affect repository performance

Concluding Remarks

IAEA's Coordinated Research Project "*The Use of Numerical Models in Support of Site Characterization and Performance Assessment Studies of Geologic Repositories*" is technically very challenging and thus required careful planning, coordination, and evaluation of intermediate results.

At this stage of its development, the CRP's overall objectives have been largely met and the coordination effort has been mostly successful, providing the basis for Phase II, in which both groups focus on the comparative analysis to arrive at conclusions regarding the value of developing alternative conceptual models, scenario selection, and parameter variation. The integration of feedback between process simulation, abstraction, and TSPA calculations will be examined.

The participants took advantage of parallel IAEA training courses in 2009 that complement the practical knowledge in applying specific codes to support this CRP.

Substantial additional training efforts (possibly supported by IAEA) and other projects or tools will be necessary for the participants to become fully proficient in the use of sophisticated simulation tools, the development of appropriate models for their respective sites, and solve their site characterization and performance assessment problems.

Acknowledgment

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