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DARIUS JUSTINAVIČIUS

Investigation of Gas Migration in a Geological Repository

Summary of Doctoral Dissertation
Technological Sciences, Energetics and Power Engineering (06T)

2014, Kaunas

KAUNAS UNIVERSITY OF TECHNOLOGY

LITHUANIAN ENERGY INSTITUTE

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Doctoral dissertation was prepared during the period of 2009–2013 at Lithuanian Energy Institute, Nuclear Engineering Laboratory.

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The dissertation is available at the Libraries of Kaunas University of Technology (K. Donelaičio g. 20, Kaunas) and Lithuanian Energy Institute (Breslaujos g. 3, Kaunas).

KAUNO TECHNOLOGIJOS UNIVERSITETAS

LIETUVOS ENERGETIKOS INSTITUTAS

DARIUS JUSTINAVIČIUS

GEOLOGINIAME ATLIEKYNE SUSIDARANČIŲ DUJŲ SKLAIDOS TYRIMAS

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1. INTRODUCTION

An international consensus exists that the geological environment is the best option for disposing of high-level radioactive waste (HLW), thus many nuclear states perform researches on implementation of such repositories. Depending on HLW management strategy, available resources and situation of the nuclear states, researches of different extents are carried out. Although currently there is none of the countries has an operating geological repository, several underground research laboratories already exist. Crystalline rocks, clay and salt formations are considered as potential environments for geological repositories. During the coming decade, at least three geological repositories will start to operate: in Finland, Sweden (crystalline rocks) and France (clay formation).

The key task of a repository is to protect people (including future generations) and environment against the negative effect of the ionizing radiation. The effect may be caused by some currently unknown repository's scenario in the long-term perspective (e. g. canister defect, earthquake, climate change, human intrusion to the repository, etc.) It must be also evaluated that implementation of nuclear waste repository will disturb stabile geological environment settled over years. HLW placed in the underground tunnels will emit residual heat and generate hydrogen gas due to corrosion of steel canisters and other structural components of the repository. Such perturbations in the geological environment induce simultaneous and coupled processes of heat transfer, fluid (liquid and gas) flow, mechanical deformation and chemical alteration. Evaluation of all these processes is a complex task that is still not solved. At the moment, particular aspects relevant to the repository's safety are evaluated in the world's practice using numerical modelling – an essential component of any radioactive waste (RW) management programme.

Relevance

Behaviour of gas generated in a geological repository is one of the particular aspects relevant to repository's safety. In a geological repository, gas may be generated due to corrosion of steel canisters and other structural components of the repository, biodegration of organic materials, radiolysis and radioactive decay. It was established that disposal packages of RW and reinforcement steel used in the construction of the repository are the principal sources of gas generation. Most intense researches on gas behaviour are carried out in those countries considering the possibility to implement a repository in the clayey formation (France, Belgium, Switzerland, United Kingdom and Canada) because concepts of such repositories intend to use steel for RW canisters and their overpacks.

During the past two decades, international projects which were held to investigate gas problem in the perspective of a geological repository safety, identified consequences of gas generation, grouped into categories according to the type of effects [1]:

- the mechanical effects on engineered and natural barriers of the repository caused by the overpressurisation if gas cannot escape through the low-permeability host rock (disruption of engineered barrier system, fracturing of the host rock);
- the direct effect of gas on groundwater flow regime around the repository (induced groundwater flow forcing the contaminated water from the canisters, migration associated with bubbles, advective flow instead of diffusion);
- the release of volatile radionuclides and toxic gas up to the biosphere.

At the present time no facts of existence of the potential risks or their possible rejection have been found, hence numerical modelling of gas migration in a geological repository is important in order to determine regularities of gas migration and to evaluate the impact of various factors on gas migration.

In Lithuania, potential environment for the geological repository is crystalline rocks and clay formation, thus gas issue is relevant. This research is closely related to problems of the Ignalina nuclear power plant decommissioning, management of RBMK-1500 spent nuclear fuel and the investigations of the possibilities to dispose it in Lithuania. The work is relevant in the aspect of competence building in the field of spent nuclear fuel disposal in Lithuania as well.

The main aim of the doctoral dissertation

The objective of the research is to perform a numerical analysis of gas migration and determine regularities of gas migration in the geological repository situated in clay formation, evaluate the impact of various factors on gas migration and gas impact on long-term safety of the geological repository.

The main tasks

1. To develop numerical models for evaluation of gas migration in a single HLW disposal cell and module (50 interconnected disposal cells) of the repository situated in clay formation.
2. To determine mechanism of gas migration, identify primary pathways of gas and estimate quantity of gas flow (in gaseous and dissolved state).
3. To estimate peak pressure of gas and its influence on the mechanical properties of the geological repository.

4. To perform sensitivity analysis of the results and evaluate factors that could possibly impact on gas migration pathways, peak pressure and quantity of gas flow (in gaseous and dissolved state).

Scientific novelty

1. Advective fluid flow through thin interfaces (primary transport pathways for gas) in the tunnels (disposal, access and main) has been taken into account for the first time in the modelling of gas migration in the geological repository.
2. Models allowing complex evaluation of advective and diffusive flow of dissolved gas and visco-capillary two-phase flow in the geological repository situated in clay formation have been developed.
3. Factors influencing peak pressure in the repository and possibly influencing its mechanical stability and functionality have been determined.

Practical importance of the dissertation

The gained experience could be used in the assessment of gas migration in a specific geological repository.

The structure and the content of the dissertation

The dissertation consists of the following chapters: introduction, analysis of the available investigations, investigation subject and methodology, results, conclusions and references. General information on the content of the dissertation is as follows: 96 pages, 47 figures, 18 tables and 82 references.

Approbation of the work

In total, 4 papers were published on the theme of doctoral dissertation. One publication has been published in the journal of Institute for Scientific Information database (ISI Web of Science) and one publication in a journal, referred in the other international databases. Two papers were published in the proceedings of international conferences.

2. INVESTIGATION SUBJECT AND METHODOLOGY

Assessment methodology of gas migration includes six parts, described in Fig. 2.1.

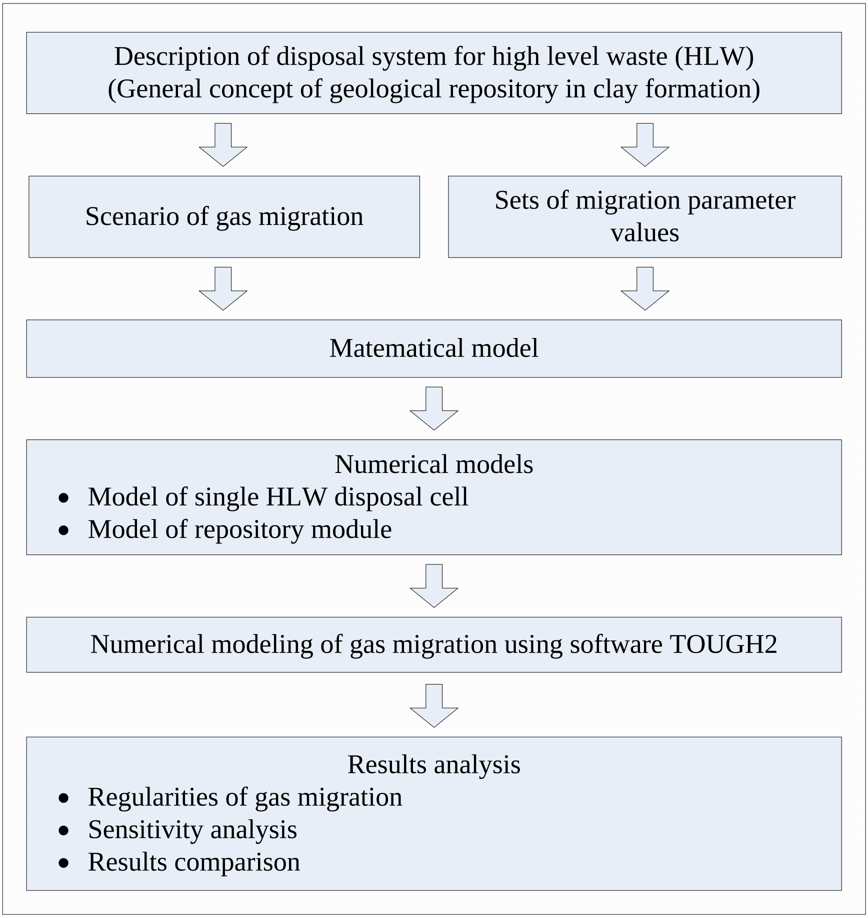

Fig. 2.1. Methodology for the analysis of gas migration in the geological repository

Investigation of gas migration was carried out using general concept of the geological repository in clay formation, which had been proposed considering the international practice. A conceptual model of gas migration was developed and gas behaviour under natural evolution scenario of the geological repository was modelled. Numerical analysis was carried out using conventional two-phase flow simulator TOUGH2. Main advantages of this software are capability to perform parallel simulations using multi-core processors and possibility to implement all thermophysical properties of hydrogen gas in the model. Two numerical models were developed in order to evaluate gas migration in the system of natural and engineered barriers. The first model represents a single HLW disposal tunnel (cell) and the second one – an HLW repository module (50 interconnected disposal cells). A sensitivity analysis was performed as well and main factors that could possibly have an impact on gas migration pathways, peak pressure and quantity of gas flow (in gaseous and liquid phase) was evaluated.

2.1. Generic repository concept for HLW disposal in clay formation

In the generic concept (Fig. 2.2), HLW containers are placed in the horizontal disposal cells situated in clay formation at a depth of about 500 m. Shaft, main and access tunnels are used for transportation of HLW. The geological repository is divided into modules on both sides of the main tunnel. Each module has 100 interconnected disposal cells that are symmetrically arranged on both sides of the access tunnel (drift). A detailed description of the module is provided in Fig. 2.3.

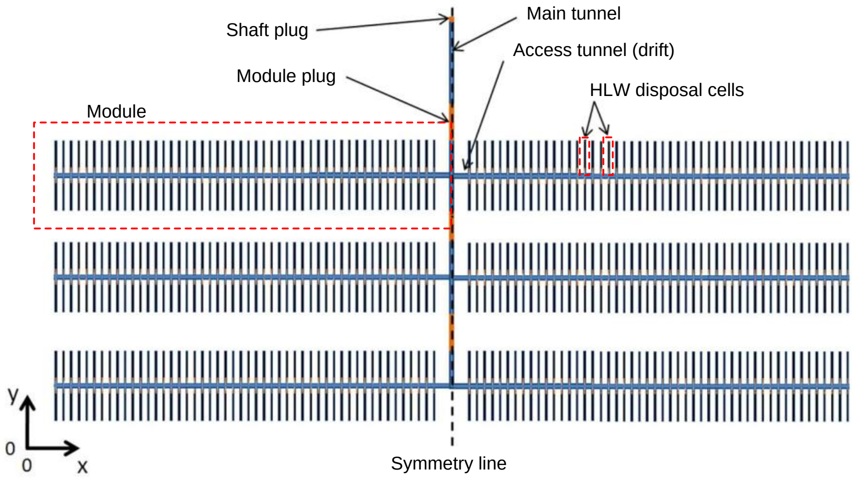

Fig. 2.2. HLW repository in clay formation; a general scheme [2]

After the placement of HLW containers, the disposal cell is sealed with bentonite. After all the disposal cells in the modules are filled with HLW, the access drifts, the main tunnel and the shaft are backfilled with mixture of bentonite and crushed clay. In order to reduce fluid outflow from the modules, they are separated from each other by 20 m long bentonite plugs as well. The same type of bentonite plug (except its length is 50 m) is placed in the shaft to prevent fluid outflow to the biosphere in case of module’s plugs failure. During the excavation, the natural geological environment around the shaft and the tunnels is disturbed, thus the engineered disturbed zone (EDZ) is a potential preferential migration pathway for fluids. Another preferential pathway for fluids' migration could be a network of thin interfaces, e. g. contact surfaces between the EDZ and (i) HLW containers in a disposal cell; (ii) bentonite plugs in the tunnels and the shaft; (iii) the backfill in the tunnels. Properties of all type of interfaces are different and depend on materials in contact.

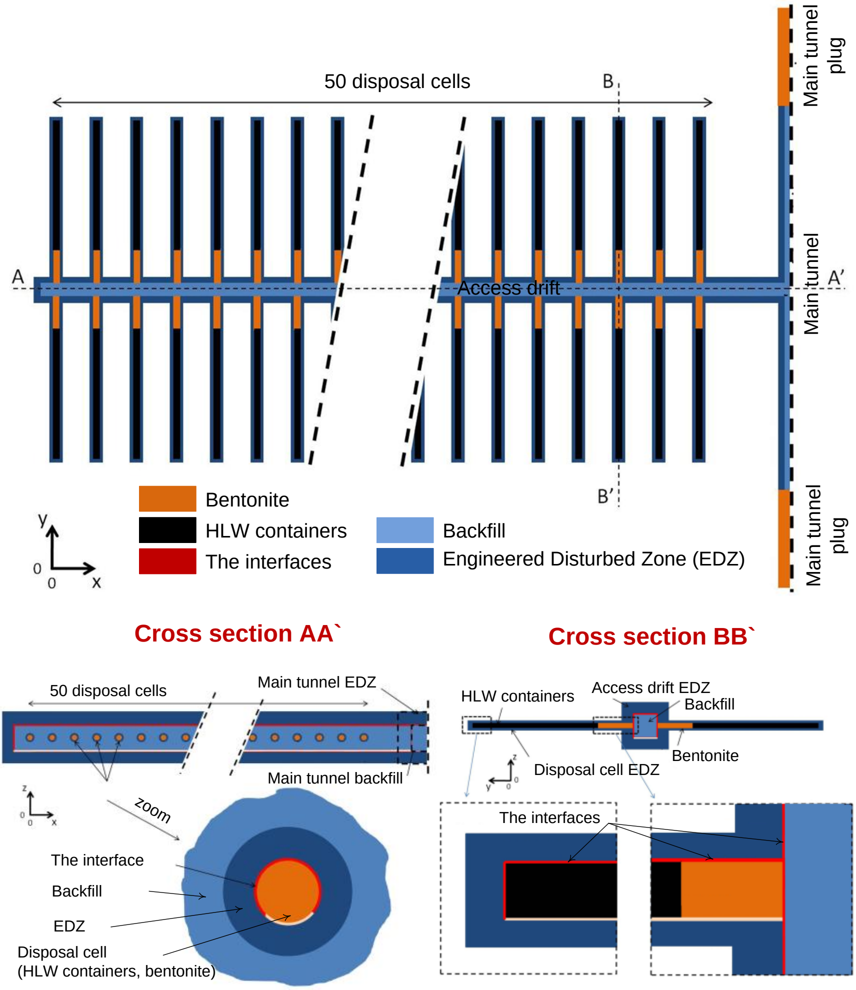

Fig. 2.3. Geological repository module [3]

2.2. Scenario of gas migration

Gas migration modelling was performed for the most probably (natural evolution) scenario of the HLW repository in clay formation. Other assumptions regarding the repository's environment were the following:

- the present climatic conditions will remain the same in the future;
- no earthquakes will occur;
- no human intrusion to the repository will happen.

According to the results of other authors [1, 4, 5], corrosion of steel canisters and of other steel components in the repository is the key source of gas generation, thus only behaviour of generated hydrogen (H_2) gas was evaluated in this study. Although the corrosion process was not modelled, it was assumed that there would be enough groundwater for corrosion reaction in the disposal cells. It was assumed that corrosion would start immediately after geological repository's closure (i. e. the engineered barrier would be unsaturated) and would proceed at the same rate in all disposal cells during the first 10,000 years. Gas generation rate was assumed to be 100 mol/year in a single disposal cell and it corresponds to ~5 μm/year steel corrosion rate. Eventual release of gaseous radionuclides after degradation of HLW containers was not modelled. Gas transport analysis was performed under isothermal conditions (20 °C temperature), i. e. residual heat removal from HLW containers was neglected since it does not influence gas migration [6]. The simulation time was limited up to 100,000 years after repository's closure.

2.3. Mathematical model

Hydrogen gas will be generated due to corrosion of disposal packages or other steel components used in the construction of a geological repository. Fluid flow in the repository involves multiphase transient flow processes. In this section mathematical model of gas migration in porous medium is described taking into account gas dissolution in groundwater, advective and diffusive flow.

The amount of gas that can be dissolved in a liquid follows Henry's law which states that at constant temperature, the mass of gas that dissolve in liquid is directly proportional to the absolute pressure of the gas [7]:

$$c = K_H \cdot P_p \quad (2.1)$$

where

- c the concentration of the solute (mol/m^3);
- K_H Henry's constant, depends on the solute, the solvent and the temperature (mol/(m^3·Pa));
- P_p the partial pressure of the solute (Pa).

Advective flow density of gas and liquid is governed by a multiphase extension of Darcy's law [7]:

$$\dot{F}_{\beta} = -k \cdot \frac{k_{r\beta} \cdot \rho_{\beta}}{\mu_{\beta}} (\nabla P_{\beta} - \rho_{\beta} \cdot g) \quad \textbf{(2.2)}$$

where

β	denotes the fluid phase (liquid or gas);
k	the intrinsic permeability (m^2);
$k_{r\beta}$	relative permeability for phase β (−);
ρ_{β}	the fluid density (kg/m^3);
μ_{β}	the coefficient of dynamic viscosity of the fluid (Pa·s);
∇P_{β}	the gradient of phase pressure (Pa/m);
g	acceleration of gravity (m/s^2);
z	the altitude of water table (m).

Diffusion process in the gas and liquid phases is described by Fick's Law and can be written as [7]:

$$\dot{F}_{\beta} = -\varphi \cdot \tau_0 \tau_{\beta} \cdot \rho_{\beta} \cdot D_{\beta} \nabla X_{\beta} \quad \textbf{(2.3)}$$

where

ϕ	effective porosity of porous medium (–);
$\tau_0\tau_{\beta}$	tortuosity which includes a porous medium dependent factor (τ_0) and a coefficient that depends on phase saturation ($\tau_{\beta} = \tau_{\beta} (S_{\beta})$);
D_{β}	molecular diffusion coefficient (m^2/s);
∇X_{β}	the gradient of fluid mass fraction.

2.4. Numerical models

2.4.1. Model of a single disposal cell

To be able to understand water and gas flow at the repository scale, it is necessary to understand water and gas flow at a cell scale (i. e. on the scale of a single disposal tunnel). The representation and geometry of a single disposal cell are shown in Fig. 2.4.

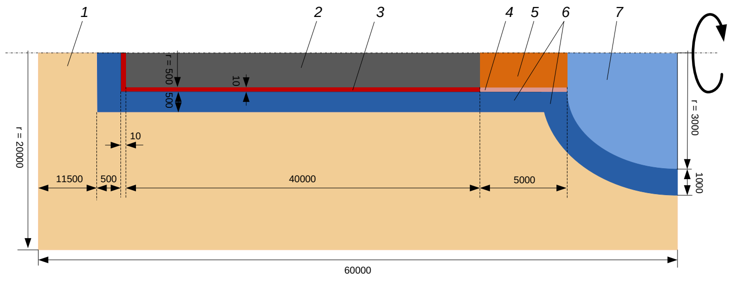

Fig. 2.4. Model of a single disposal cell: 1 – undisturbed clay formation; 2 – HLW containers; 3 – waste interface; 4 – bentonite plug interface; 5 – bentonite plug; 6 – engineered disturbed zone (EDZ); 7 – access drift

A two-dimensional disposal cell model in a cylindrical r-z system was developed and analyzed. As the scale is quite small (few tens of meters), it was possible to represent fine geometric features and especially the interfaces. Both interfaces were considered as centimetre-thick regions and were represented with one layer of grid elements. The modelling domain was meshed with 4,836 rectangular grid elements (Fig. 2.5) and was refined in engineered materials due to higher gradients of the physical variables and a finer result resolution required.

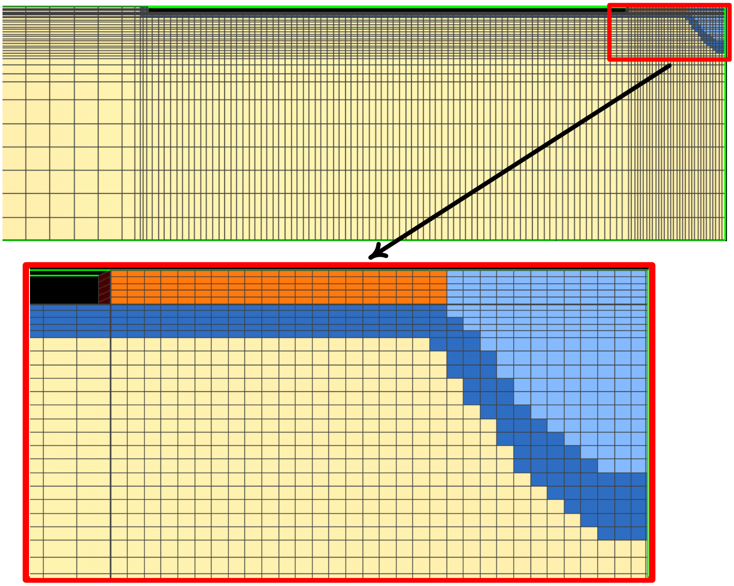

Fig. 2.5. Computational grid of a disposal cell model

Since the HLW containers are constituted of a material impermeable to liquid and gas flow, they were not explicitly represented in the model. Hydrogen gas was injected directly to the interface between the HLW containers and the EDZ. The constant pressure (5 MPa) condition at the outer radial boundary and time varying boundary conditions (gas pressure and gas saturation) at the outer boundary of the access drift were assumed in the model. All other boundary conditions were designated as no-flow. Initial gas saturation was set to be 0.3 in the bentonite plug and the access drift and 0.95 in both interfaces. The remaining part of the modelling domain was assumed fully water saturated. Initial groundwater pressure was set to be 5 MPa in all water saturated parts of the model (according to a continuous formulation, the gas and water pressures are the same if there appears only dissolved gas). In other parts of the model gas pressure was set to be 0.1 MPa.

2.4.2. Model of the repository module

The repository module consists of two parts with 50 cells on each side of the access drift (Fig. 2.3). Due to the mirror boundary along the centre of the access drift, a model of only half module was developed. The modelling domain was three-dimensional and was meshed with 90,000 rectangular grid elements (Fig. 2.6). Initial conditions in the module were the same as in a single disposal cell model, except the initial pressure in water saturated materials, which varies linearly from 6 MPa at the bottom to 4 MPa at the top of the model. Time varying boundary conditions were implemented at the outer boundary of the main tunnel.

2.5. Modelling

Hydrogeodynamical modelling is an assessment of groundwater flow regime and of dissolved chemical (hydrogen gas in this case) in flowing groundwater by solving differential equations. International researches showed that one of the leading software's to evaluate gas migration is TOUGH2 developed in Lawrence Berkeley National Laboratory (USA). TOUGH2 is a numerical simulator for non-isothermal flows of multicomponent, multiphase fluids in one, two and three-dimensional porous and fractured mediums [8]. However, this software is not user friendly due to complicated pre-processing and post-processing. Input and results files in TOUGH2 are provided as text files, thus additional tools are necessary to prepare and process this data. In this dissertation, TOUGH2 graphical interface PETRASIM [9] and language of technical computing MATLAB were used to prepare the input data and process the results.

The EOS5 fluid property routine was selected for the description of thermophysical properties of hydrogen gas. The components that the geological repository contains were assumed to be a three phase porous medium, consisting of solid skeleton, pore-liquid and pore-gas. In this case groundwater (κ_1) and hydrogen gas dissolved in groundwater (κ_2) was considered as liquid phase (β_1) while hydrogen gas (κ_3) and water vapour (κ_4) was considered as gas phase (β_2). The TOUGH2 solves mass balance equation by the integrated finite difference method. The basic equation solved by TOUGH2 can be written in general form [8]:

$$\frac{d}{dt}\int_{V_n} M^{\kappa} dV_n = \int_{\Gamma_n} F^{\kappa} \cdot n d\Gamma_n + \int_{V_n} f^{\kappa} dV_n \qquad (2.4)$$

where

V_n an arbitrary sub-domain of the flow system;
Γ_n the surface bounded two arbitrary sub-domains;
n a normal vector on surface element $d\Gamma_n$;

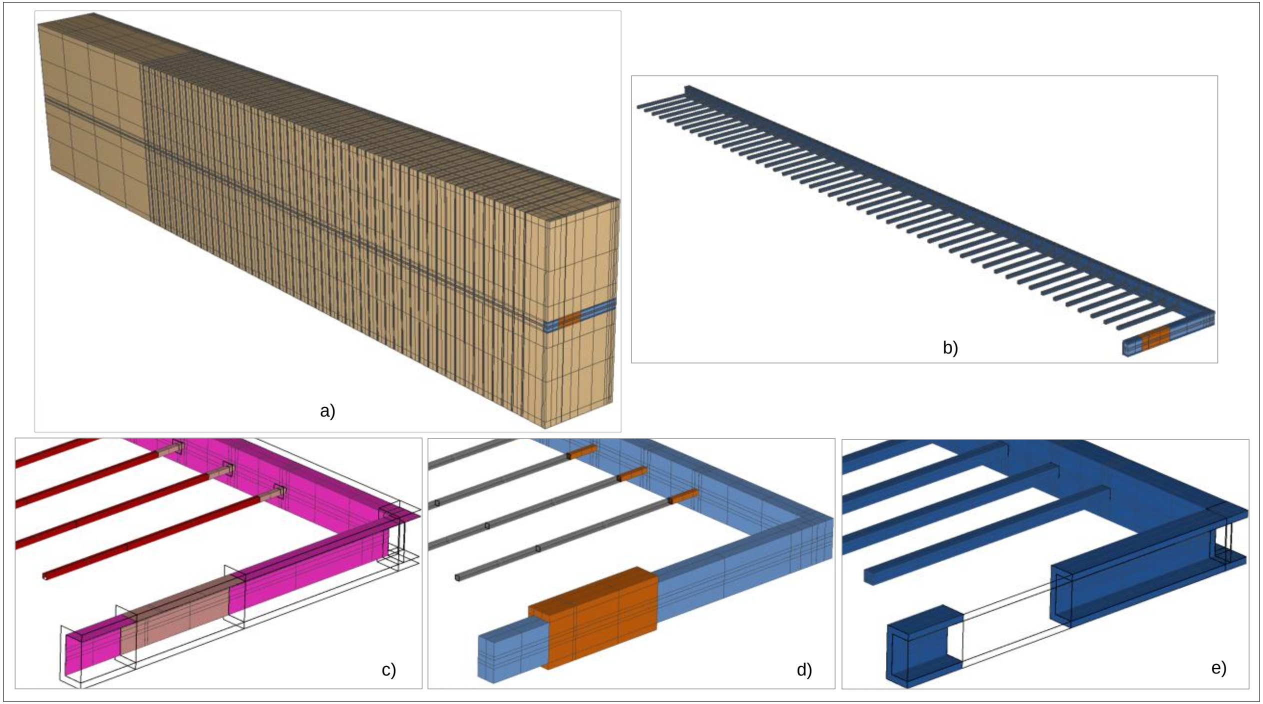

Fig. 2.6. Computational grid of the repository module coloured by material type: a) full modelling domain; b) system of the tunnels and the EDZ; c) interfaces; d) engineered barriers; e) the EDZ

M^κ the mass of component κ (kg);

F^κ advective and diffusive flow density of component κ, calculated according to 2.2 and 2.3 equations (kg/(m^2·s));

f^κ the source term of each component κ (kg/s).

As the model of the repository's module is very complex and numerical analysis is time-consuming, gas migration modelling in the module was performed using parallel version of TOUGH2 (TOUGH2-MP) [10].

2.6. Results analysis

The key results allowing evaluating gas migration regularities in the geological repository are: gas saturation in porous medium S_g, peak pressure in analysed system P_g and gas (in gaseous and dissolved state) flow from the gas source (steel containers) to the biosphere.

2.6.1. Regularities of gas migration

To evaluate regularities of gas migration in a single disposal cell, variation of the results (S_g, P_g) were analysed in the observation points (Fig. 2.7). Point P2 is in the interface between the HLW containers and the EDZ, points P3 and P4 are in the interface between bentonite plug and the EDZ, points P5, P6 and P7 are in different places of the EDZ, P1 and P8–P11 are in different places of undisturbed clay formation.

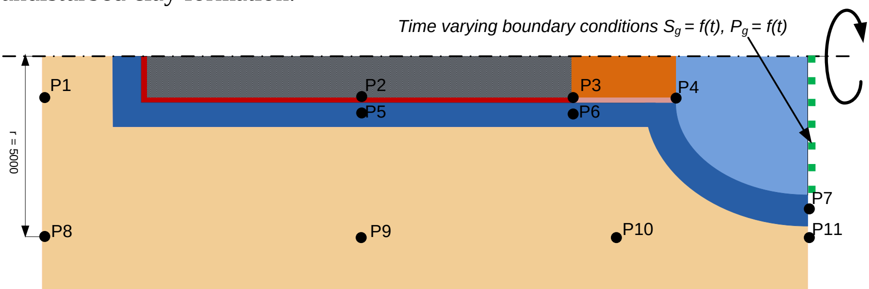

Fig. 2.7. Observation points in a single disposal cell model

Fluxes of gaseous and dissolved hydrogen were evaluated through different surfaces (shown in Fig. 2.8): between both interfaces (S-int1), an interface facing the plug and the access drift (S-int2), the EDZ near the disposal containers and the EDZ near the bentonite plug (S-EDZ), the access drift and the surrounding medium (S-drift), disturbed and undisturbed clay formations (S-clay) and through outer boundaries of the model: in the access drift (S-drift(out)) and in undisturbed clay formation (S-out).

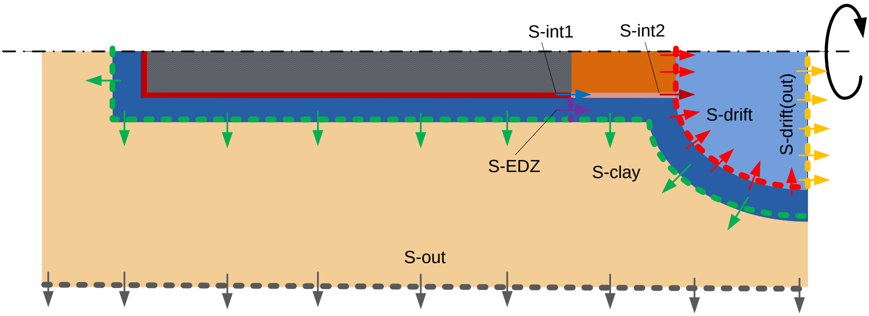

Fig. 2.8. Observation surfaces and directions of fluid fluxes in a single disposal cell model

To evaluate regularities of gas migration in the repository module, variation of the results (S_g, P_g) were analysed in the observation points (shown in Fig. 2.9) of three tunnels – disposal (DT), access (AT) and main (MT). Point P1 is in clay formation 5 m away from the disposal cell, P2 is in the interface of a disposal cell between the HLW containers and the EDZ, P3 is in the interface of the access drift between the backfill and the EDZ, P4 is in the interface of the main tunnel between the bentonite plug and undisturbed clay formation and P5 is in the bentonite plug of the main tunnel, TVBC – time varying boundary conditions implemented in the main tunnel beyond the bentonite plug.

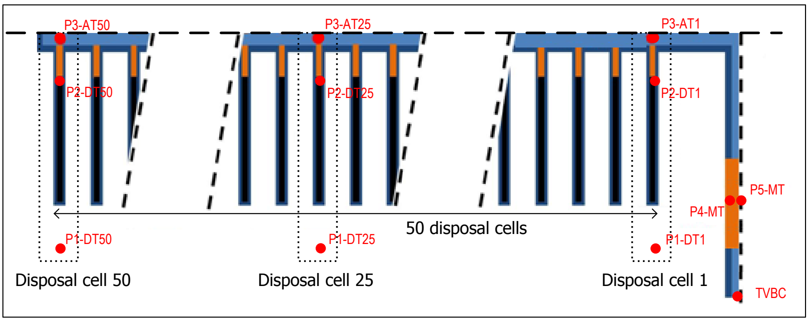

Fig. 2.9. Observation points in the repository module model

Concerning transport of gaseous hydrogen, the following fluxes through analysed surfaces (Fig. 2.10) were evaluated: from different disposal cells (section of an interface and the EDZ) to the access drift through surfaces S-DT1, S-DT25, S-DT50, from the access drift (section of the backfill, an interface and the EDZ) towards the main tunnel through surfaces S-AT1, S-AT25, S-AT50 and out of a plug of the main tunnel (section of bentonite and the interface) through surface S-MT. Transport of dissolved hydrogen through the upper (S-UP) and the lower (S-LOW) boundaries of the model was also evaluated.

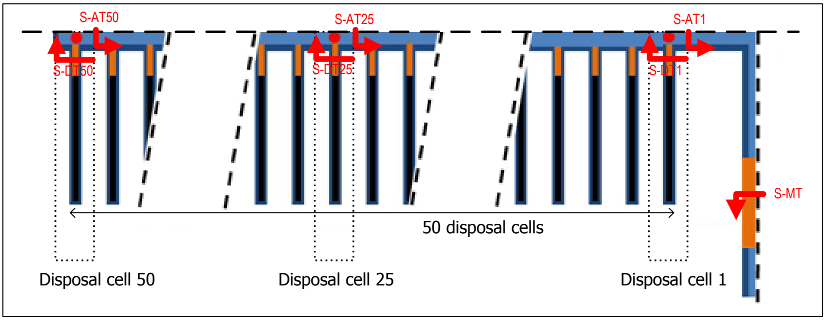

Fig. 2.10. Observation surfaces and directions of fluid fluxes in the repository module model

2.6.2. Results sensitivity analysis

Modelling of gas migration is a complex task where processes in the system are described by differential or integral equations, which are solved by numerical methods. Solution of this task requires a lot of time and computer resources, thus uncertainty and sensitivity analysis could not be performed using probabilistic methods. Uncertainty analysis in a single disposal cell model was performed using a local sensitivity analysis method. In this case influence of one parameter's uncertainty was evaluated for the results. Using this method, only several additional runs of the model (using the lowest and the highest values of the parameter) were sufficient. Parameters evaluated using local sensitivity analyses were ranked according to their importance (numerical value of the sensitivity index) to the result. Tornado plots, in which the data categories are listed vertically, and the categories are ordered so that the largest bar appears at the top of the chart that was drawn.

Gas migration in the geological repository could be influenced by the characteristics of natural and engineered barriers (value of intrinsic permeability *k*, model of relative permeability k_r function, temperature), characteristics of diffusion process (tortuosity model, values of molecular diffusion coefficient), features of corrosion process (start, duration, rate), characteristics of the disposal system (e. g. evaluation of interfaces) or features of the numerical model (boundary conditions, numerical aspects). All sensitivity cases analysed in this dissertation are summarized in Table 2.1.

In order to compare the results of the thesis with the results of other authors, they were submitted to numerical modelling section of recent EU-F7 research project FORGE.

Table 2.1. Description of analyzed sensitivity cases

	Description
1. Characteristics of disturbed and undisturbed clay	
S11	**Less permeable EDZ**. Intrinsic permeability of the EDZ is supposed to be equal to undisturbed clay permeability ($k_{S11} = 1 \cdot 10^{-20}$ m^2)
S12	**More permeable EDZ**. Increasing the intrinsic permeability value of the EDZ from the nominal value of $k_{nom} = 1 \cdot 10^{-17}$ m^2 to $k_{S12} = 1 \cdot 10^{-16}$ m^2
S13	**Altered relative permeability curve**. Van Genuchten – Mualem relative permeability function was changed to Fatt and Klikoff function for clay formation and the EDZ
2. Characteristics of interfaces	
S21	**Less permeable waste interface**. Decreasing the intrinsic permeability value of the waste interface from the nominal value of $k_{nom} = 1 \cdot 10^{-12}$ m^2 to $k_{S21} = 1 \cdot 10^{-15}$ m^2
S22	**More permeable plug interface**. Increasing the intrinsic permeability value of the plug interface from the nominal value of $k_{nom} = 1 \cdot 10^{-17}$ m^2 to $k_{S22} = 1 \cdot 10^{-16}$ m^2
S23	**Model without waste interface**. Waste interface have the same properties as the EDZ
S24	**Model without plug interface**. Plug interface have the same properties as bentonite
S25	**Model without both interfaces**. The characteristics of waste interface are the same as the EDZ and characteristics of the plug interface are the same as the bentonite plug
3. Characteristics of tunnel backfill	
S31	**Less permeable backfill.** Decreasing the intrinsic permeability value of backfill from the nominal value of $k_{nom} = 5 \cdot 10^{-17}$ m^2 to $k_{S31} = 5 \cdot 10^{-18}$ m^2
S32	**More permeable backfill.** Increasing the intrinsic permeability value of backfill from the nominal value of $k_{nom} = 5 \cdot 10^{-17}$ m^2 to $k_{S32} = 5 \cdot 10^{-16}$ m^2
4. Influence on temperature	
S41	**System is isothermal (10 °C temperature)**
S42	**System is isothermal (30 °C temperature)**
5. Characteristics of diffusion	
S51	**Alternative tortuosity model**. "Millington-Quirk" expression instead of "Relative permeability" model for tortuosity was used
S52	**Increased diffusion**. Molecular diffusion coefficient of dissolved hydrogen under water saturated conditions multiplied by 10: $D_{H2\_S52} = 4.6 \cdot 10^{-8}$ m$^2 \cdot$s
S53	**Decreased diffusion**. Molecular diffusion coefficient of dissolved hydrogen under water saturated conditions divided by 10: $D_{H2\_S53} = 4.6 \cdot 10^{-10}$ m$^2 \cdot$s
S54	**Model without diffusion**. Only advective mass transport was considered
6. Characteristics of corrosion	
S61	**Gas generation delay for 10 years**
S62	**Gas generation delay for 100 years**
7. Influence on boundary conditions	
S7	**Model without time varying boundary conditions**. No flow boundary conditions assumed for access drift boundary
8. Influence on numerical aspects	
S81	**Higher convergence tolerance**. Increasing value of relative convergence criterion in TOUGH2 from the nominal value of $1 \cdot 10^{-4}$ to $1 \cdot 10^{-5}$
S82	**Lower convergence tolerance**. Decreasing value of relative convergence criterion in TOUGH2 from the nominal value of $1 \cdot 10^{-4}$ to $1 \cdot 10^{-3}$

3. RESULTS AND DISCUSSION

3.1. Evaluation of gas migration in a single disposal cell

3.1.1. Reference case results

Reference case (deterministic) analysis of gas migration in a single disposal cell was carried out using nominal (most reasonable) values of the parameters according to [11]. Graph of gas saturation at observation points (Fig. 2.7) in which gas phase evolves is presented in Fig. 3.1. Time varying boundary condition (TVBC) implemented at the outer boundary of the access drift is presented in this figure as well.

Analysis of the modelling results showed that significant levels of gas saturation were reached in both interfaces. The interfaces were almost fully desaturated, but the evolution of gas saturation depends on the position of a particular observation point. The interface near waste containers (point P2) was resaturated up to ~0.15 – ~0.2 from ~5 up to ~1,000 years due to the water inflow from the surrounding clay. Due to gas generation in this interface, gas builds-up and completely pushes water away after ~4,000 years. Similar evolution was observed at a point between both interfaces (P3). The evolution in the interface near the bentonite plug (P4) was different: within first ~4 years the interface becomes fully gas saturated and remains such till the end of gas generation. Full resaturation in both interfaces (at points P2, P3 and P4) was reached after ~11,000 years after repository closure.

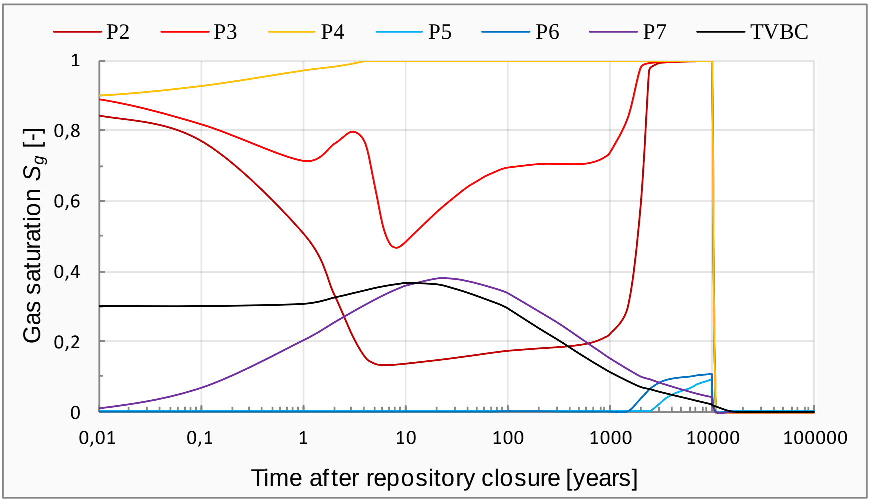

Fig. 3.1. Evolution of gas saturation at the observation points

Gas saturation in the EDZ never exceeds 12 % and exists only for particular time periods: in the cell EDZ (P5) from ~2,500 up to ~11,000 years, in the bentonite plug EDZ (P6) from ~70 up to ~350 and from ~1,400 up to ~11,000 years and in the drift EDZ (P7) evolution of gas saturation is very closely linked to implemented time varying boundary condition at the drift boundary. Full resaturation in the backfill of the access drift (P7) was reached after ~20,000 years after repository closure. Gas saturation in undisturbed clay formation never exceeds 3 % and exists only in contact with drift EDZ. Free gas was not observed in the undisturbed clay 5 m away from a disposal cell (at points T1, T8–T11). Only hydrogen gas dissolved in groundwater were detected in undisturbed clay formation. Dissolved gas diffuses towards the outer radial boundary due to concentration gradient.

As it could be seen in Fig. 3.2, the peak pressure of ~5.7 MPa was observed in the interfaces (at points P2 and P3) and the EDZ (at points P5 and P6). The peak overpressure due to gas was reached at the end of the corrosion process and exceeded initial (hydrostatic) pressure in the disposal cell by ~15 %. However, such pressure is much lower than lithostatic pressure (~10 MPa) in the selected geological repository concept, thus mechanical effects on engineered and natural structures of the repository caused by the pressure build-up that may follow from gas generation are not presumable. These results also showed that Darcy, Fick and Henry laws are sufficient to describe gas behaviour in a single disposal cell and continuous fluid flow approach realized in TOUGH2 could be used.

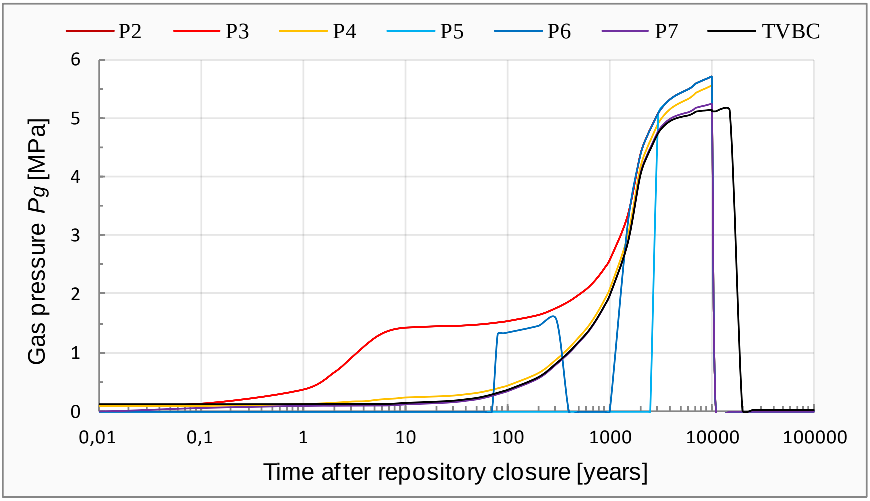

Fig. 3.2. Evolution of gas pressure at the observation points

Graph of gaseous hydrogen flux through different surfaces (Fig. 2.8) is presented in Fig. 3.3. Positive flow rate indicates H_2 flow towards the access drift. Gas generation rate in a single disposal cell is presented in this graph as well. The results showed that hydrogen was transported from the disposal cell towards the access drift during the period of gas generation (up until 10,000 years). Most of generated hydrogen (~85 %) flows towards the access drift and major part of this hydrogen (~81 %) flows through the very thick interface (surface S-int1). Remaining part (~4 %) flows through the EDZ (surface S-EDZ). As hydrogen access to the plug interface, whose permeability is much lower (equal to permeability of the EDZ), part of this hydrogen (~49 %) flows through the plug interface (surface S-int2) and the remaining part (~24 %) flows towards the drift through the EDZ. Overall, ~73 % of the generated hydrogen was transported from a disposal cell toward the access drift in gaseous form while the remaining part is dissolved in pore-water and diffuses in undisturbed clay formation. Gaseous hydrogen that enters the access drift (surface S-drift) instantly leaves it through the lateral side of the drift boundary (surface S-drift(out)).

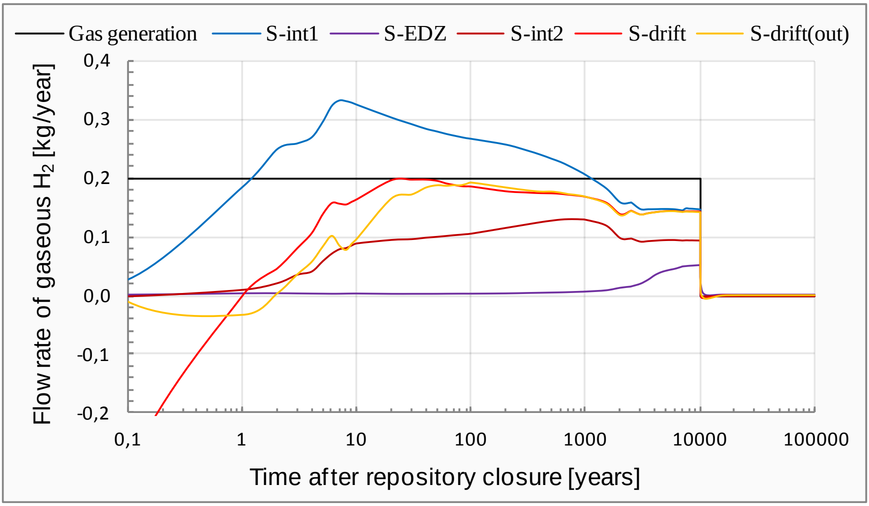

Fig. 3.3. Evolution of gaseous H_2 flux through different surfaces

Advective flow is the primary transport mechanism of gaseous hydrogen during gas generation period (Fig. 3.4). The diffusion process has a significant impact on gaseous hydrogen transport only during the first hundreds of years. Diffusive flow is the primary transport mechanism of the dissolved hydrogen into clay formation.

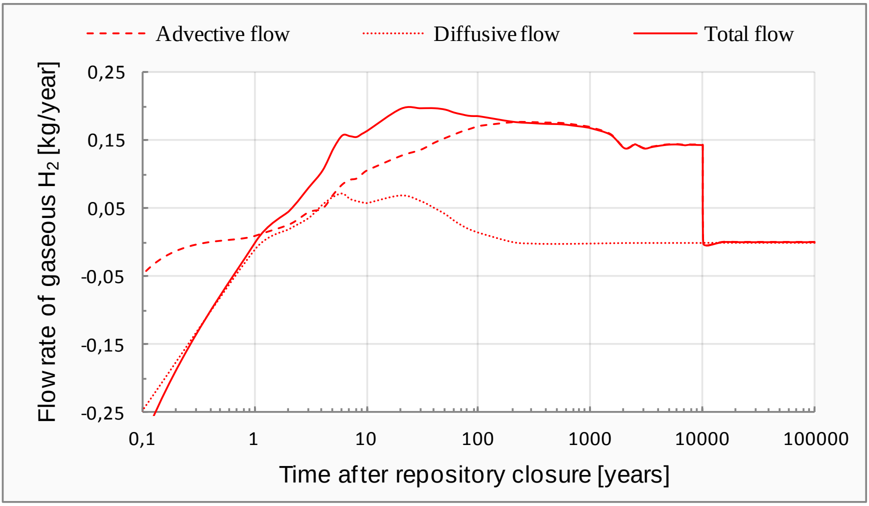

Fig. 3.4. Evolution of gaseous H_2 flux towards the access drift

In the first part of the final FORGE report [12], description of computer softwares used for modelling of each team, main assumptions and deviations from task specification [11], analysis and comparison of achieved results are presented. The conclusions state that the results of three authors (among nine participants) cannot be compared due to limitation of the used software. Meanwhile, the software used by LEI allowed evaluating the necessary processes (gas dissolution in groundwater, advective and diffusive flow of dissolved gas and visco-capillary two-phase flow). The graphs in this report show that LEI results correlate well with results of the other authors.

3.1.2. Results sensitivity analysis

The estimated peak pressure was 5.7 MPa in the reference case model. Sensitivity analysis results of the peak pressure are shown in Fig. 3.5. The highest pressure (12.7 MPa) was identified in the model without time varying boundary conditions (S7). Such model does not represent the basic concept of the geological repository as a single disposal cell is not an isolated system but a part of the repository's tunnel system. In this case, the lithostatic (geological environment) pressure in the repository would be exceeded and the gas generated due to corrosion would become dangerous to mechanical stability and functionality of the geological repository. While selecting materials for the geological repository, it is essential to consider that they should not cause blocking of gaseous H_2 flow from a disposal cell to the system of the repository's tunnels (i. e. materials of lower porosity and permeability are not advisable for the backfill).

There were three more cases sensitive to pressure increase, compared to the reference case results – less permeable EDZ (S11) and models without considering both (S25) or only waste (S23) interface. The reference case results have shown that the EDZ and interfaces are preferential pathways for gaseous H_2 flow from the disposal cell to the access drift. If the permeability of these materials decreases, the amount of gas transferred towards the access drift also decreases, i. e. the gas accumulates around the disposal cell and the pressure increases. The peak pressure at such cases exceeds the reference result 27 % − 16.3 % but it does not exceed the lithostatic pressure of the geological formation (~10 MPa) by its absolute values (7.3 MPa − 6.6 MPa).

Evaluating pressure decrease, compared to the reference case results, it is essential to indicate the cases of increased diffusion (S52), more permeable EDZ (S12) and more permeable backfill (S32).

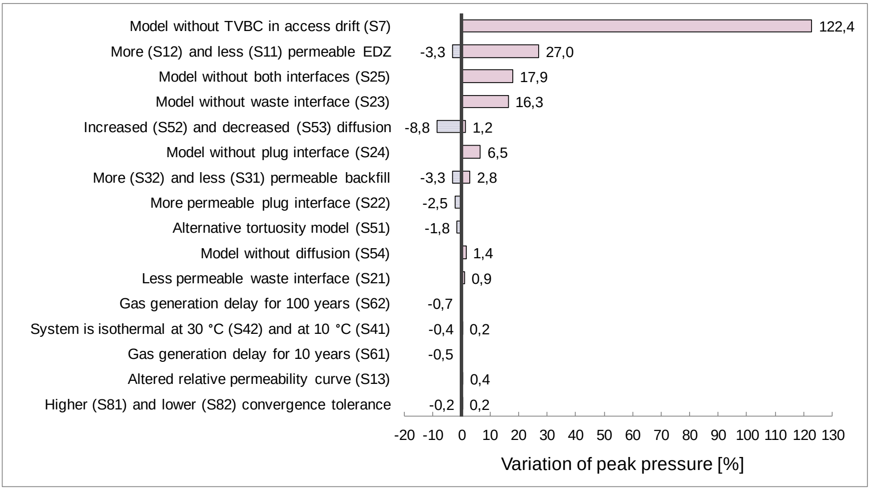

Fig. 3.5. Comparison of peak pressure in the system for all analysed cases

Comparing sensitivity of gaseous H_2 flux to the access drift (Fig. 3.6), it was determined that the highest variations are related to diffusion process, especially to uncertainty of molecular diffusion coefficient of dissolved hydrogen. The difference of molecular diffusion coefficient by two orders of magnitude determines transport of all generated hydrogen only by diffusion (in dissolved state) to the clay formation (S52) or transfer of most of the generated H_2 by convective flow towards the access drift (S53). The results are opposite in models neglecting time varying boundary condition (S7) and diffusion process (S54). In the first case, gaseous H_2 is not transported towards the access drift due to implemented no-flow boundary condition in the lateral side of the drift boundary (all generated H_2 flows towards the disturbed and undisturbed clay formation). In the second case, all generated H_2 is transported towards the access drift by convective flow.

Decreased flux of gaseous H_2, compared to the reference case results, was also determined in cases of alternative tortuosity model (J51), of higher temperature (S42) and in models without considering both (S25) and only waste (S23) interface. A little higher flux of gaseous H_2 towards the access drift, compared to the reference case was determined in cases of lower temperature (S41) and less permeable EDZ (S11).

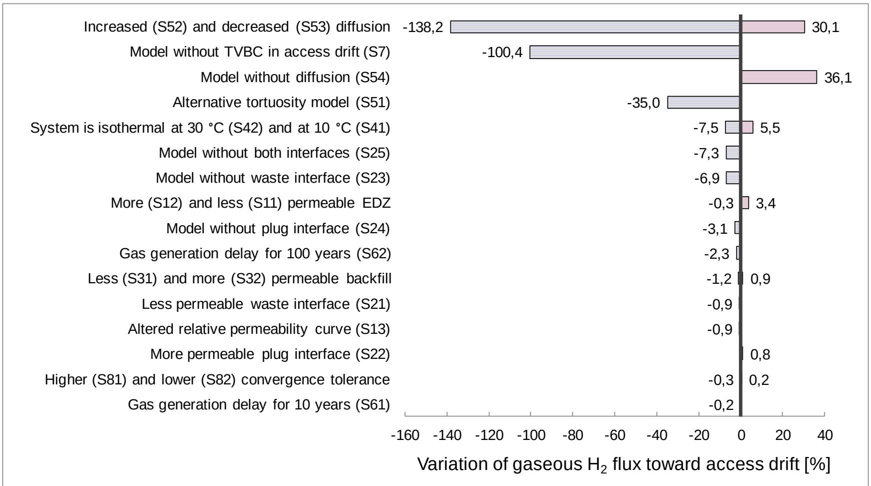

Fig. 3.6. Comparison of gaseous H_2 flux towards the access drift for all analysed cases

Comparing the amounts of the dissolved H_2 flowing through the outer radial boundary (Fig. 3.7), it was determined that characteristics of diffusion process, evaluation of interfaces and uncertainty of EDZ permeability have the highest influence on these results. The amount of the dissolved H_2 flowing through the outer radial boundary is inversely proportional to the amount of the gaseous H_2 flowing towards the access drift.

Analysis of all sensitivity cases showed that the results of gas migration are weakly (< 2 %) sensitive to reduced permeability of the waste interface (S21), altered relative permeability curve in disturbed and undisturbed clay formation (S13), gas generation delay for 10 and 100 years (S61, S62) and value of convergence tolerance in TOUGH2 (S81, S82).

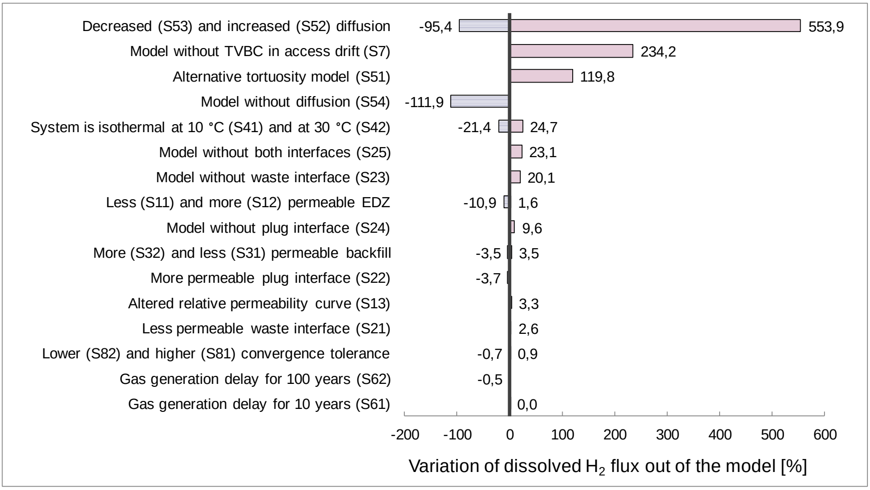

Fig. 3.7. Comparison of dissolved H_2 flux out of the model for all analysed cases

3.2. Evaluation of gas migration in the repository module

Evaluation of gas migration in the repository module was performed using nominal values of the parameter (the same as in the reference case of a single disposal cell model). Graph of gas saturation at the observation points (Fig. 2.9) in which gas phase evolves is presented in Fig. 3.8. Time varying boundary condition (TVBC) implemented at the outer boundary of the main tunnel backfill is presented in this graph as well.

Evolution of gas saturation in the interfaces near HLW containers (P2-DT) is similar to the case of a single disposal cell (see Fig. 3.1). The lowest saturation during gas generation period was ~0.3 in module case while the lowest saturation in a disposal cell model was ~0.15. In both models, these interfaces were fully gas saturated after ~4,000 years and remain such till the end of gas generation. A little different evolution of gas saturation in waste interfaces of particular disposal tunnels (points P2-DT1, P2-DT25 and P2-DT50) could be explained by higher potential of groundwater inflow from the surrounding clay formation receding from the main tunnel. All waste interfaces became fully water saturated at a similar time, i. e. after ~16,000 years after repository closure.

The interface in the access drift between the backfill and the EDZ (P3-AT) was fully gas saturated after ~500 years and remains such till the end of gas generation. Full resaturation of this interface occurs after ~20,000 years after repository closure. Since saturation evolution was the same in different points (P3-AT1, P3-AT25, P3-AT50) of the interface (520 m length), it could be concluded that gas was transported rapidly by convective flow in this interface.

Gas saturation in the interface of the main tunnel's plug (P4-MT) increased from ~0.95 to ~0.99 in the first 12,000 years after repository closure. Considering the fact that the bentonite plug (P5-MT) was fully water saturated after ~5,000 years due to time varying boundary condition implemented at the outer boundary of the main tunnel backfill, it could be concluded that the interface (P4-MT) was not resaturated because of the gas inflow there from module.

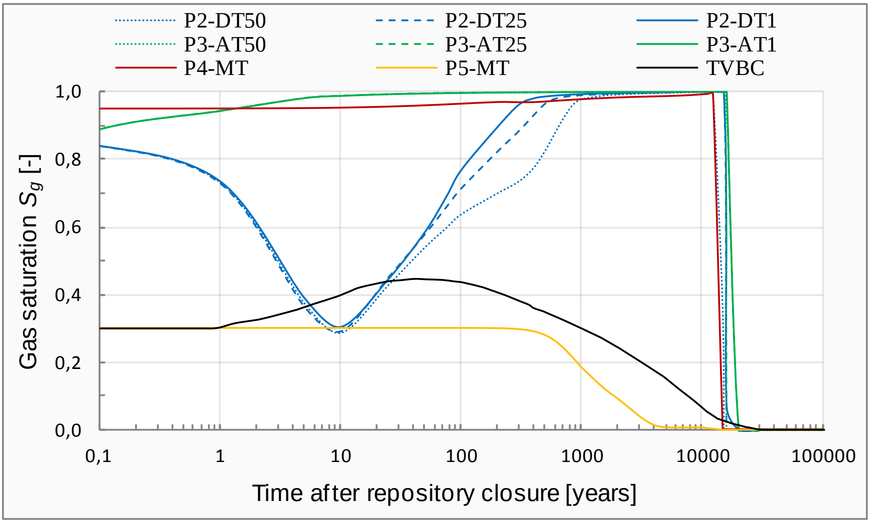

Fig. 3.8. Evolution of gas saturation at the observation points

Evaluating gas pressure in the module (Fig. 3.9), it was determined that the highest pressure was reached in the waste interfaces of the disposal tunnels (at points P2-DT1, P2-DT25 and P2-DT50) and in the interfaces of the access tunnels (at points P3-AT1, P3-AT25 and P3-AT50). Evolution of gas pressure in the interface (P4-MT) and the bentonite plug (P5-MT) of the main tunnel was very similar. The pressure profiles were in-between the pressure in the module and time varying boundary condition implemented at the outer boundary of the main tunnel backfill. Thus, it could be concluded that time varying boundary condition controlled the pressure in the bentonite plug and the plug controlled the pressure in the module. The determined peak pressure in the module (and in any disposal cell) was ~8 MPa and did not exceed the lithostatic pressure (~10 MPa) of the selected geological repository concept.

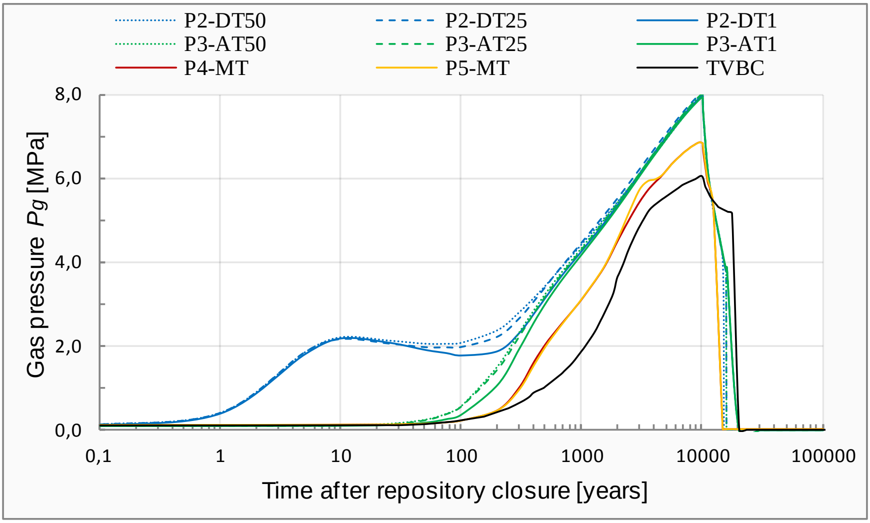

Fig. 3.9. Evolution of gas pressure at the observation points

Graph of gaseous hydrogen flux through different surfaces (Fig. 2.10) is presented in Fig. 3.10. Positive flow rate indicates H_2 flow towards the access drift and the main tunnel. Gas generation rate in a single disposal tunnel is presented in this graph as well.

Analysis of gaseous H_2 flow in the module shows that most of gas generated in disposal cells was transported towards the access drift (through surfaces S-DT1, S-DT25 and S-DT50) in the first hundreds of years after repository closure. For this reason pressure in the access drift increased and gaseous hydrogen flow out of the disposal cells decreased (gas build-up). Gas pressure in the disposal tunnels was reduced due to dissolution of hydrogen gas and diffusion of dissolved hydrogen towards the surrounding clay formation. The efficiency of diffusion process depends on circulation of groundwater which is faster receding from the main tunnel. It can be seen analysing the profile of gaseous H_2 flux through surface S-DT50. In this case, gaseous H_2 started to flow back in the disposal cell after ~2,000 years after repository closure because of higher pressure in the access drift. It can be seen analysing the flux of gaseous H_2 in the access drift (see flux through surface AT) as well. The gaseous H_2 flux toward the main tunnel (S-AT1) was a little higher, compared to the flux out of the module through the bentonite plug (S-MT). This flux decreased while receding from the main tunnel (S-AT25). At the end of the access drift (S-AT50), the flux direction changed and gaseous H_2 was transported towards the disposal cells. Transport of gaseous H_2 stopped after ~16,000 years after repository closure.

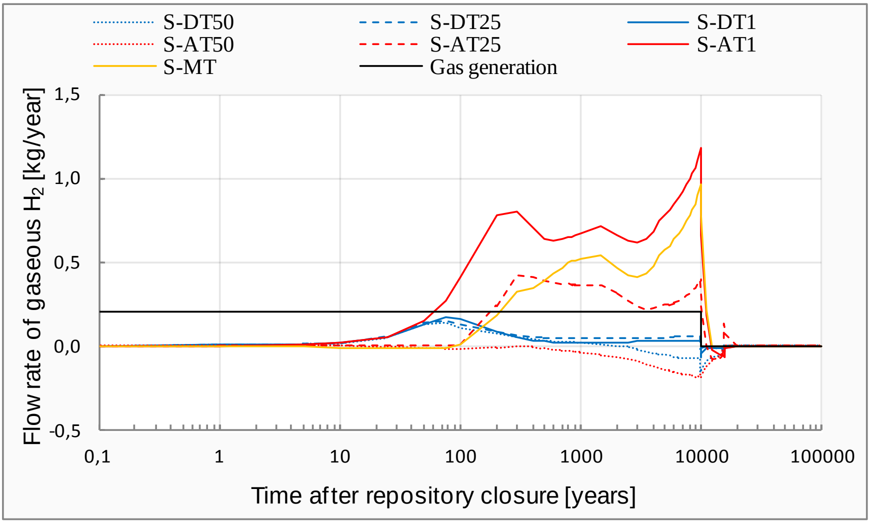

Fig. 3.10. Evolution of gaseous H_2 flux through different surfaces

It was also determined that ~10 % of gas generated in a single disposal cell was transported to the access drift through surface S-DT1, ~25 % – through surface S-TD25 and ~ –37 % – through surface S-TD50. ~8.5 % of gas generated in the module was transported towards the main tunnel through surface S-AT1 and ~6.7 % of it was transported out of the module through the bentonite plug (S-MT). The remaining part of the generated gas dissolved in groundwater and diffused into the surrounding clay formation. The dissolved H_2 reached the upper and the lower boundaries of the model (distance of 75 m) almost at the same time – 1,000 years after repository closure. ~94 % of gas generated in the module dissolved and diffused out through these surfaces.

The results of gas migration modelling in the repository module were submitted to EU-F7 research project FORGE as well. Conclusions of the second part of the final report [13] indicate that six teams (including LEI) successfully performed gas migration modelling in three-dimensional model. The graphs in this report show that LEI results correlate well with the results of the other authors.

CONCLUSIONS

The complex and systematic analysis of hydrogen gas (generated due to corrosion of steel containers) migration in a single disposal cell and a module (50 interconnected disposal cells) of a conceptual geological repository situated in clay formation at 500 m depth was carried out. Advective fluid flow through thin interfaces in the tunnels was taken into account in numerical models. Based on modelling results, regularities of gas migration were determined, the impact of various factors on gas migration and gas impact on long-term safety of the geological repository was evaluated and the following conclusions were determined:

1. In reference case, most of the generated hydrogen (~73 %) is transported by advective flow from the disposal cell towards the access drift. Primary pathways for gaseous hydrogen are interfaces and engineered disturbed zone (EDZ). Approx. 49 % of gaseous H_2 flows through interfaces and ~24 % flows through the EDZ. The remaining part of the gas dissolves in the groundwater and diffuses towards the undisturbed clay formation.
2. The peak pressure in the analysed models (under the reference and local sensitivity cases) does not exceed the lithostatic (geological environment) pressure in the repository, thus is not sufficient to disturb the mechanical stability and functionality of the engineered barriers system.
3. It was determined that no macrofractures were created in the repository's materials, thus diffusive and advective flow of the dissolved gas and visco-capillary two-phase flow are sufficient mechanisms to describe gas behaviour in the geological repository in clay formation.
4. The highest variation of peak pressure, compared to the reference case result, were determined in the case of less permeable EDZ (+27 %) and in the models without considering both (+18 %) or only waste interface (+16 %) in the disposal tunnel.
5. The highest influence on gaseous hydrogen flux towards the access drift, compared to the reference case result, has characteristics of diffusion process: uncertainty of molecular diffusion coefficient, evaluation of diffusion process and alternative tortuosity model.
6. The highest influence on dissolved hydrogen flux towards the undisturbed clay formation, compared to the reference case result, has characteristics of diffusion process: uncertainty of molecular diffusion coefficient, evaluation of diffusion process, alternative tortuosity model and temperature in the model.

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PUBLICATIONS RELATED TO THE DISSERTATION

Publication in the journal of Institute for Scientific Information database (ISI Web of Science)

1. Justinavičius, Darius; Narkūnienė, Asta; Poškas Povilas. Impact of different factors on gas migration in the disposal cell of conceptual geological repository for high level radioactive waste. *Mechanika*. Kaunas University of Technology, Lithuanian Academy of Sciences, Vilnius Gediminas Technical University. Kaunas: KTU. ISSN 1392-1207. 2012, Vol. 18, no. 6, p. 650–656. [Science Citation Index Expanded (Web of Science); INSPEC; Compendex; Academic Search Complete; FLUIDEX; Scopus].

Publication in the journal, referred in the other international databases

1. Justinavičius, Darius; Poškas, Povilas. Gas migration modelling in the disposal cell of conceptual geological repository for high-level radioactive waste. *Power Engineering*. Lithuanian Academy of Sciences. Vilnius: Press of Lithuanian Academy of Sciences. ISSN 0235-7208. 2012, Vol. 58, no. 2, p. 97–107. [Academic Search Complete; IndexCopernicus, INSPEC] (in Lithuanian).

Publications in conference proceedings

1. Justinavičius, Darius. Modelling of two-phase flow of hydrogen gas in the disposal cell of repository for high level radioactive waste. In *Proceedings of the 9th International Conference of Young Scientists on Energy Issues CYSENI 2012*, May 24–25, 2012, Kaunas, Lithuania. Kaunas: LEI. ISSN 1822-7554. 2012, p. 658–667.
2. Justinavičius, Darius. Influence of porous medium permeability on gas migration in the disposal tunnel of conceptual geological repository. In *Proceedings of the 10th International Conference of Young Scientists on Energy Issues CYSENI 2013*, May 29–31, 2013, Kaunas, Lithuania. Kaunas: LEI. ISSN 1822-7554. 2013, p. 651–658.

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Darius Justinavičius was born on December 9, 1981 in Šiauliai. He graduated from Vilkija secondary school in 2000 and in the same year became a student of Kaunas University of Technology. He completed the studies of Applied Physics at the Faculty of Fundamental Sciences in 2004 and obtained Bachelor’s degree in Physics. Two years later, he completed the studies of Medical Physics at the same faculty and obtained Master’s degree in Biophysics. Since 2008, he has been working at the Nuclear Engineering Laboratory of the Lithuanian Energy Institute. In 2009, he became a Ph.D student in the field of Energetics and Power Engineering. During the whole period of his doctoral studies he has also worked as a junior researcher at the Nuclear Engineering Laboratory. His professional and scientific knowledge has been extended in the training courses in the United Kingdom, Czech Republic and France.

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REZIUMĖ

Branduolinė energetika, kaip ir kitos pramonės šakos, gamina ne tik naudingą produkciją, bet ir atliekas. Branduolinės atliekos, kurių santykinis tūris žymiai mažesnis, palyginti su kitų pramonės šakų atliekomis, yra radioaktyvios, todėl kelia ypatingą pavojų aplinkai ir žmonėms. Ne visos radioaktyviosios atliekos yra vienodai pavojingos žmogui, todėl skirstomos į kategorijas. Kiekvienos rūšies atliekos yra tvarkomos skirtingai, kuo jos pavojingesnės, tuo šalinamos giliau, o atliekyno konstrukcija patikimesnė. Pavojingiausias, t. y. ilgaamžes vidutinio ir didelio aktyvumo atliekas (taip pat ir panaudotą branduolinį kurą) rekomenduojama dėti į geologinius atliekynus, įrengtus giliai po žeme tam tinkančioje stabilioje geologinėje aplinkoje.

Svarbiausia geologinio atliekyno paskirtis – žmonių (ir ateities kartų) bei aplinkos apsauga nuo neigiamo jonizuojančiosios spinduliuotės poveikio. Šis poveikis gali atsirasti dėl šiuo metu nežinomo atliekyno raidos scenarijaus ateinančiais tūkstantmečiais (pvz., pažeisto konteinerio, žemės drebėjimo, klimato kaitos, žmogaus įsibrovimo į atliekyną ir pan.). Taip pat reikia įvertinti, jog geologiniuose sluoksniuose įrengtas atliekynas sutrikdys stabilią, per ilgus amžius nusistovėjusią geologinę aplinką. Požeminiuose tuneliuose patalpinti radioaktyviųjų atliekų konteineriai ne tik emituos likutinį šilumos kiekį, bet ir išskirs vandenilio dujas dėl plieninių konteinerių ir kitų atliekyno konstrukcinių komponentų korozijos. Šie pokyčiai geologinio atliekyno aplinkoje lems kartu vykstančius ir tarpusavyje susijusius šilumos mainų, fluidų (vandens ir dujų) pernašos, mechaninius ir cheminius procesus. Kompleksinis visų šių procesų įvertinimas yra sudėtingas uždavinys, kuris kol kas nėra išspręstas. Pasaulinėje praktikoje, pasitelkiant modeliavimą, kuris yra labai svarbi radioaktyviųjų atliekų tvarkymo programos dalis, vertinami atskiri atliekyno saugai svarbūs aspektai.

Vienas iš šių aspektų yra geologiniame atliekyne susidarančių dujų elgsena. Daugiausia tyrimų šioje srityje vyksta šalyse, kuriose analizuojamos galimybės atliekyną įrengti molingoje aplinkoje, kadangi tokių atliekynų koncepcijose numatomos plieninės radioaktyviųjų atliekų pakuotės ir jų apvalkalai. Lietuvoje potencialiomis aplinkomis geologiniam atliekynui įrengti laikomos kristalinės ir molingosios uolienos, o dujų sklaidos analizė neatlikta. Šis darbas glaudžiai susijęs su RBMK-1500 panaudoto branduolinio kuro iš Ignalinos AE galutinio sutvarkymo Lietuvoje galimybių tyrimais o taip pat aktualus kompetencijos plėtojimo aspektu.

Šiame darbe, atlikus skaitinę dujų sklaidos analizę, nustatyti susidarančių dujų sklaidos dėsningumai geologiniame atliekyne, įrengtame molingoje aplinkoje, įvertinta įvairių veiksnių įtaka sklaidai ir dujų įtaka ilgalaikei geologinio atliekyno saugai.

Modeliuojant dujų sklaidą geologinio atliekyno patalpinimo tunelyje ir modulyje (50-yje sujungtų patalpinimo tunelių), pirmą kartą atsižvelgta į konvekcinę pernašą siaurais tunelių inžineriniais tarpeliais. Sukurti modeliai leidžia kompleksiškai įvertinti difuzinę ir konvekcinę vandenyje ištirpusių dujų bei klampią-kapiliarinę dvifazio (vanduo ir dujos) srauto pernašą. Nustatyti veiksniai, lemiantys didžiausią slėgį atliekyne ir galintys turėti įtaką jo mechaniniam stabilumui ir funkcionalumui.

Pagrindiniai darbe gauti rezultatai parodė, kad maksimalus vandenilio dujų, susidarančių dėl plieninių didelio aktyvumo radioaktyviųjų atliekų konteinerių korozijos, slėgis patalpinimo tunelio ir modulio modeliuose, išnagrinėtais baziniu ir lokalios jautrumo analizės atvejais, neviršija litostatinio (geologinės aplinkos) slėgio 500 m gylyje, todėl yra nepakankamas, kad sutrikdytų mechaninį inžinerinių barjerų sistemos stabilumą ir funkcionalumą. Kadangi atliekyno medžiagose nesukuriami makroplyšiai, todėl difuzinė ir konvekcinė vandenyje ištirpusių dujų ir klampi-kapiliarinė dvifazio srauto pernaša yra pakankami mechanizmai apibūdinant dujų elgseną geologiniame atliekyne, įrengtame molingose uolienose. Didžiausias slėgio padidėjimas modelyje, lyginant su baziniu atveju, nustatytas esant mažesniam skvarbos koeficientui kasimo sutrikdytoje zonoje (+27 %) ir nevertinant abiejų (+18 %) arba vieno (+16 %) inžinerinio tarpelio patalpinimo tunelyje. Didžioji dalis (~73 %) susidarančio dujinio vandenilio sklinda konvekciniu būdu nuo radioaktyviųjų atliekų patalpinimo tunelio gabenimo tunelio link. Pirmenybiniai sklaidos keliai – inžineriniai tarpeliai, kuriais pernešama ~49 % ir kasimo sutrikdyta zona, kuria pernešama ~24 % susidariusio dujinio vandenilio. Likusi susidariusių dujų dalis ištirpsta požeminiame vandenyje ir difuzijos būdu pernešama į kasimo nesutrikdytą molingąją aplinką. Iš patalpinimo tunelio pasišalinančio dujinio vandenilio pokytį labiausiai veikia difuzinę pernašą lemiantys veiksniai – molekulinės difuzijos koeficiento neapibrėžtumas, difuzijos proceso neįvertinimas ir alternatyvus porų vingiuotumo parametro modelis. Iš patalpinimo tunelio pasišalinančio vandenyje ištirpusio vandenilio pokytį labiausiai veikia difuzinę pernašą lemiantys veiksniai – molekulinės difuzijos koeficiento neapibrėžtumas, alternatyvus porų vingiuotumo parametro modelis, difuzijos proceso neįvertinimas ir temperatūra analizuojamoje sistemoje.

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