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UNSATURATED ZONE MODELS AND THEIR APPLICATION FOR RADIOACTIVE WASTE REPOSITORY SAFETY ANALYS

Summary of doctoral dissertation
Physical Sciences, Geology (05P)

Vilnius, 2013

The dissertation research was carried out at the Nature Research Centre, Institute of Geology and Geography in 2009–2012.

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The official defense of the dissertation will be held at the public meeting of the Physical Science Council on November 12, 2013, at 15:00. in the main hall of the Institute of Geology and Geography. Address: Ševčenkos 13, LT 03223, Vilnius, Lithuania.

The summary of the dissertation was distributed on 10 October, 2013.
The dissertation is available at the libraries of Vilnius University and Institute of Geology and Geography, Nature Research Centre.

VILNIAUS UNIVERSITETAS
GAMTOS TYRIMŲ CENTRO
GEOLOGIJOS IR GEOGRAFIJOS INSTITUTAS

Žana Skuratovič

AERACIJOS ZONOS MODELIAI IR JŲ TAIKYMAI RADIOAKTYVIŲJŲ ATLIEKŲ KAPINYNO SAUGOS ANALIZEI

Daktaro disertacijos santrauka
Fiziniai mokslai, geologija (05P)

Vilnius, 2013

Disertacija rengta 2009–2012 metais Gamtos tyrimų centro Geologijos ir geografijos institute.

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Disertacija bus ginama viešame Geologijos mokslų krypties tarybos posėdyje 2013 m lapkričio 12 d. 15 val. Geologijos ir geografijos instituto didžiojoje salėje Adresas: T. Ševčenkos 13, LT 03223, Vilnius, Lietuva.

Disertacijos santrauka išsiuntinėta 2013 m. spalio 10 d.
Disertaciją galima peržiūrėti Geologijos ir geografijos instituto ir Vilniaus Universiteto bibliotekose.

Introduction

Scientific and technological progress produces chemical and radioactive wastes, which can get into the environment. Fertilizers, pesticides, pharmaceutical products and hormone residues in combination with pathogenic microorganisms are inserted into the environment consistently by agricultural activity; organic compounds, salt, accidental spill of toxic trace elements from industrial and municipal waste landfills, particularly in urban areas, and also radioactive waste generated by nuclear technology. Being of variable origin, many of these substances can enter biogeochemical cycles of the ecosystems and create health risks, especially when they enter the food chain through the surface and ground water. Radioactive waste safety issues have become especially relevant for the countries with nuclear energy. Solutions of these issues focus on the surface repository with the natural and engineered barriers.

In recent decades, the soils of unsaturated zone are regarded as the first natural barrier to a large extent able to limit the spread of contaminants. Over time, radionuclides from the radioactive waste storage facilities and repositories can reach and contaminate the ground water aquifer through the unsaturated zone.

In Lithuania, low and intermediate level radioactive wastes, generated by medical, industrial and research activities, were accumulated at the Maišiagala radioactive waste repository. Short lived low and intermediate level radioactive wastes, generated during the operation of the Ignalina Nuclear Power Plant (INPP) and after the dismantling of INPP will be stored at the repository near the Ignalina NPP. Following the studies of the geological conditions in the territory of Lithuania, the Ignalina NPP region has been assessed as the most appropriate location for the repository construction. Disposal of radioactive waste is the last step in the chain of waste management.

In order to assess the possible effects of radioactive contamination on the groundwater system, and for the prediction of the radioecological impacts, mathematical modelling studies for the radionuclide migration from the repository through the unsaturated zone under different scenarios are required.

In the analysis of the flow and transport processes in the soil, numerical methods for solving various differential equations have started to be used widely when high speed computers were created. Mathematical modelling tools to predict the water and the solute movement between the ground and the water table surfaces are available. However the problem of the model calibration based on experimental data often remains unsolved, especially dealing with scenarios for the planned facilities.

Unsaturated zone is an important part of water circulation cycle and an integral part of many hydrological and hydrogeological factors and processes. Seeking for solutions, analysis and prediction of the process demand appropriate steps.

In this study, the computer program HYDRUS was used and examined in more detail. The program allows analyzing soil properties of engineering materials and their changes under the influence of rainfall, evaporation, vegetation cover, and many other environmental factors and processes.

The aim of the study

There were two aims of the study: 1) to characterize two sites of nuclear facilities with different hydrogeological conditions; 2) to identify the unsaturated zone soils moisture and solute transport processes and evaluate their performance characteristics.

The object of investigation

Experimental and modelling techniques were applied to study the unsaturated zone processes of the nuclear facility sites, determining the first natural barrier to the ground water saturation processes and solute transport through unsaturated zone.

The research methods:

The research methods include experimental and observational studies of the unsaturated zone and numerical simulations of moisture and solute transport.

The main tasks of doctoral dissertation:

1. Selection and optimization of the unsaturated zone experimental research, monitoring and modelling methodology.
2. Collection and analysis of undisturbed and disturbed soil samples of the unsaturated zone.
3. Performing tests and analysis to determine soil physical–mechanical properties and hydraulic conductivity values of the unsaturated zone profile.
4. Systematic monitoring of ground water level; monthly precipitation amount; analysis of the isotopic (tritium, oxygen-18 and deuterium) composition of groundwater, precipitation and the unsaturated zone moisture.
5. Construction of the unsaturated zone models, based on *in situ* tests and laboratory experiments; comparison of the unsaturated zone moisture profiles and radionuclide composition.

Originality of the results

There have been no long-lasting and detailed unsaturated zone experimental research and numerical analysis in Lithuania. For the first time, the globally widespread radionuclide tritium (^{3}H) and isotopic tracers ratio (δ^{18}O and $\delta\ ^2$H) distribution features were determined in precipitation, unsaturated zone soil moisture profiles and groundwater. The transport processes through the unsaturated zone have been modelled and analyzed by numerical models.

Positions to be defined

Resulting from global processes, stable isotope and tritium seasonal variation in precipitation, in the unsaturated zone and especially in groundwater are averaged over time and almost disappear; traces of seasonal peaks are recognizable only in case of rapid infiltration occurrence.

Moisture and solute transport through unsaturated zone is under the control of the soil physical mechanical properties, heterogeneity, and variation of the hydraulic properties; the existence of less permeable soil layers even of very small thicknesses creates natural barrier, limiting moisture and solute transfer.

Based on complex isotopic studies, it is possible to calibrate the numerical models through the unsaturated zone and reduce the uncertainty of predicted results.

Extent and structure

The doctoral dissertation includes introduction, 3 main chapters, conclusions, and references. The dissertation comprises 138 pages, 48 figures and 16 tables.

Acknowledgements

I am grateful to Prof. Habil. Dr. Jonas Mažeika for scientific guidance and support. I am grateful to Dr. Petras Klizas for the possibility to use experimental equipment and support. Hearty thanks are given to Dr. Saulius Gadeikis, Julija Vaitkevičienė, Elvyra Bulavkaitė, Juozas Kapeckas for advices and help. I am grateful to Tõnu Martma for providing stable isotope data. Hearty thanks to Dr. Vaidotei Jakimavičiutė–Maselienė, Dr. Rimantas Petrošius and Dr. Algirdas Zuzevičius for reviewing the dissertation manuscript.

Special thanks go to Radioactive Waste Management Agency for providing data and possibility to work at the Maišiagla radioactive waste repository site.

The State Studies Foundation and the Research Council of Lithuania are worth special thanks for financial support.

SHORT CONTENT OF THE DOCTORAL DISSERTATION

1. Literature review

Radioactive waste is produced by nuclear power generation during the operation of nuclear reactors, nuclear fuel production cycle, research, health care institutions and industrial companies. The near surface radioactive waste repositories in many countries are used for solid and solidified very short lived, low and intermediate level radioactive waste disposal. Investigations have shown that this type of waste disposal is a safe waste isolation option. Well constructed repositories are an efficient and effective way for safe isolation of radioactive wastes. Safety assessment plays the central role in the development of a near surface repository which has different purposes at various stages of development, operation and closure of a repository. At an early stage, safety assessments should be used to determine the feasibility of disposal concepts, to direct site investigations and to help in initial decision making.

Surface water can be contaminated with radionuclides from a disposal facility thought groundwater discharge to surface runoff. The unsaturated zone is the first natural barrier which could be encountered with radionuclides release from a disposal facility. Various analytical solutions can be used to solve the advection–dispersion transport. Mathematical models are a tool for studying unsaturated zone flow and transport processes. While certain problems may be solved using relatively simple analytical models, other problems require more sophisticated numerical models that simulate water flow, solute transport and a range of biogeochemical reactions.

In recent years, the unsaturated zone has been expected to act as a barrier for possible transport of contaminants to groundwater. Since the infiltrating water flow depends on the natural percolation at the site and the performance of engineered barriers, modelling of unsaturated water flow is required.

Due to natural events and human activities over the time, the system characteristics change according to scenarios. Scenarios consider natural phenomena, i.e. gradual or sudden change of conditions, which, over time can affect repository safety. Scenario analysis requires the identification and interpretation of the events that may initiate or increase the release of radionuclide into the environment. During safety assessment period additional data collection is possible, which focuses on certain parameters, which are necessary to ensure the safety of the repository (Yim et al., 2000). Since the beginning of operation of the Ignalina NPP, radioactive wastes were stored within the plant. The wastes can not be stored there for long time. They should be placed in the constructed repositories suitable for storing the waste for an indefinite period of time. The location for radioactive waste repository was approved based on the results of environmental impact assessment, performed geological investigations, favourable social and economic conditions. The selected site is located in the territory of Visaginas municipality, namely the Stabatiškė site, in close vicinity to the Ignalina NPP (Paviršinio..., 2007).

Moisture transport features in the unsaturated zone

The unsaturated zone is characterized by porous system where pore spaces are not fully saturated with water. Due to capillary effects in pores, water pressure in the unsaturated zone is less than the atmospheric pressure. The unsaturated zone provides a linkage between atmospheric moisture, groundwater, and seepage of groundwater to streams, lakes, or other surface water bodies. The major difference between water flow in saturated and unsaturated soils is that the coefficient of permeability (hydraulic conductivity), which is conventionally assumed to be a constant in saturated soils, is a function of degree of saturation or matrix suction in the unsaturated soils. The pore water pressure generally has a negative gauge value in the unsaturated region, whereas the pore water pressure is positive in the saturated zone. Despite the differences, the formulation of the partial differential flow equation is similar in the two cases. With the dependence of unsaturated hydraulic conductivity *K(h)* on water potential or water content, Darcy’s law is written in the following form (Sposito, 1986), which is called Buckingham-Darcy law:

$$q = -K(h)\frac{\partial H}{\partial z} = -K(h)\frac{\partial (h+z)}{\partial z} = -K(h)\left(\frac{\partial h}{\partial z}+1\right). \qquad (1)$$

Isotopic studies of the unsaturated zone and water systems

Since 1961, the Global Network of Isotopes in Precipitation (GNIP) has provided the isotopic observations of precipitation worldwide. The GNIP network is a survey of oxygen and hydrogen isotope contents in precipitation, including oxygen-18 (^{18}O), deuterium (^{2}H) and tritium (^{3}H). The entire GNIP database is available to the public for viewing and can be downloaded from the IAEA website (www.iaea.org/water).

Environmental tracer techniques (^{3}H, δO^{18}, $\delta^{2}H$) are being increasingly used to evaluate flow processes. Variations of stable isotopes in water can give important information on unsaturated zone processes such as infiltration, evapotranspiration, mixing and recharge.

Zimmermann et al. (1967) worked on observation of the behaviour of isotopes in porous materials. This work was extended to unsaturated zone by Munnich et al. (1980) and Allison (1982). In the early 1980s, Fontes worked on changes in the isotopic composition of soi1 water in deep unsaturated zones in the Sahara. Barnes and Allison (1988) reviewed the work on the behaviour of isotopes in the unsaturated zone. Maloszewski et al. (1995) used ^{18}O and ^{2}H in rainfall to study percolation through refuse.

In Lithuania, isotopic studies of water bodies had been done before the construction of Ignalina NPP, a follow–up was carried out after the construction and since 1978 isotope monitoring of the water bodies has been performed off and on. Also groundwater isotope studies have been carried out during the research for the planned Visaginas NPP. Tritium concentration studies not only in groundwater but also in surface water bodies – in rivers and lakes, the Baltic Sea, Curonian Lagoon – and continuous measurements of precipitation have been carried out, as well.

Numerical models of unsaturated zone

Mathematical models become indispensable tools for studying unsaturated zone flow and transport processes. While certain problems may be solved using relatively simple analytical models, many problems require more sophisticated numerical models that simulate water flow, solute transport and a range of biogeochemical reactions.

The majority of currently available unsaturated zone models are based on either the Richards equation (Richards, 1931) or the kinematic wave equation (Colbeck, 1972; Smith, 1983; Smith, Hebbert, 1983). While the Richards equation considers flow due to both capillary and gravity forces, the kinematic wave equation neglects capillarity and considers only gravity. Modelling of unsaturated zone flow processes, however, is a complex and computationally demanding task that is often handicapped by the lack of data necessary to characterize the hydraulic properties of the subsurface environment.

The finite element method is used as an alternative to the finite difference method, especially for problems in which the model boundaries are irregular and/or for problems in which the porous medium is heterogeneous or anisotropic. Disadvantages of finite element methods are numerical oscillation, instability, and larger computation time.

2. Methods

Unsaturated zone studies were carried out in different regions of Lithuania in terms of hydrogeological situation: in the Maišiagala radioactive waste storage facility area, where homogeneous sand soil dominates, and in the Stabatiškės near surface repository site for low and intermediate level short lived radioactive waste, where unsaturated zone profile is heterogeneous and consists of combination of sand and clay soils. The Maišiagala radioactive waste storage facility is set up in the Bartuškis forest, 7 km from Maišiagala town and 40 km from Vilnius. The Quaternary glacial deposits occur on the top of sedimentary cover settled by glacier melt water and consisting of sand, gravel, pebble, loam and sandy loam. The thickness of the Quaternary formation is 100–120 m (Juodkazis, 1979). The aeolian fine grained sands are present in the region with the thickness exceeding 10 m.

The Stabatiškė near surface repository site is located in the recharge area of the eastern part of the Baltic artesian basin. It is in the territory of Visaginas municipality, in close vicinity to the Ignalina Nuclear Power Plant (NPP). This location was approved based on the results of environmental impact assessment. The thickness of Quaternary deposits in the region varies from 62 to 260 m. The shallow groundwater is located in peat, sand, gravel, cobbles and pebbles, the fissured upper part of the eroded sandy glacial till, and the lenses of sand and gravel within the till deposits (Marcinkevicius et al., 1995).

The main experimental and observational tasks include the collection of undisturbed and disturbed soil samples; determination of the physical properties and the hydraulic conductivity values of soil samples, moisture extraction from the soil sample for isotopic studies; observation of the groundwater dynamics at the Maišiagala piezometer; groundwater sampling for isotopic analysis (^{3}H, δ^{18}O, δ^{2}H) once in a month; and monthly precipitation isotopic analysis (Vilnius and Zarasai).

Soil density was determined by using a ring of known volume and upon extraction the soil core within the ring was dried to determine the mass of solids and water present at the time of sampling.

Gravimetric water content was measured by drying sample in an oven at 105º C; the dry soil sample was then weighed and soil moisture content was calculated.

Hydraulic conductivity laboratory tests of the soil samples were performed at the laboratory of Vilnius University by the falling head method.

Grain size distribution was determined through sieve and hydrometric analyses which were performed by Dr. Saulius Gadeikis and Julija Vaitkevičienė.

To perform pore water extraction for isotopic analyses, a moisture extraction system was designed to extract water from the unsaturated core samples without any isotopic fractionation. Flask containing soil sample is connected to a vacuum line at the entry of the extraction system. The moisture traps are cooled to -196ºC using liquid nitrogen. The flask containing sample is gradually heated at 95ºC. The soil moisture was extracted using vacuum distillation, the groundwater samples and precipitation samples were analyzes for the beta decay counting.

The beta decay counting of ^{3}H was run for a 12 ml of scintillation cocktail and 8 ml of water electrolytically enriched with ^{3}H. ^{3}H specific activity was determined by the liquid scintillation counter TRI-CARB 3170TR/SL and Quantulus-1220 at the Radioisotope

Research Laboratory of Nature Research Centre. As the extracted moisture from soil samples only amounted to a few ml, the specific activity of the ^{3}H was determined by direct measurement (without enrichment), in which the uncertainty can reach 2–4 TU. Since the monthly precipitation and monthly groundwater sampling volume was 600 ml and sufficient to perform the enrichment of ^{3}H, the specific activity of ^{3}H was determined by measuring electrolytically enriched water with ^{3}H; in this case, the uncertainty can reach only 0.1–0.2 TU.

^{18}O/^{16}O and ^{2}H/^{1}H ratios of water molecules were determined as δ^{18}O and δ^{2}H values with respect to international standard (VSMOW) (Coplen, 1996). The investigations were carried out using IRMS DELTA V Advantage and GasBench II system or Picarro L2120-i Cavity Ring-Down Spectrometer. Stable isotopes data are presented as per mille deviations from internationally accepted standards with the reproducibility of ±0.1‰ for δ^{18}O and ±1‰ for δ^{2}H. Stable isotopes ratio measurements were performed at the Laboratory of Isotopes Palaeoclimatology at the Institute of Geology of Tallinn University of Technology, Estonia.

Both sites were modelled by using unsaturated flow and transport model of HYDRUS-1D (Šimunek et al., 2008). HYDRUS-1D is a very flexible model to express the unsaturated zone and provide numerically stable solutions. HYDRUS-1D (Šimunek et al., 2008) is a finite element code to simulate the water, solute and heat transport through unsaturated zone. Since it is capable to consider the variety of physical and chemical conditions and processes, it is widely used in unsaturated zone hydrology for many applications including the performance assessment of the waste disposal areas.

The HYDRUS computer code uses the non-linear Richards equation to solve numerically unsaturated water flow in the porous media. The soil retention characteristics and unsaturated hydraulic conductivity under changing water content are the basic soil properties required by HYDRUS. To determine soil hydraulic properties, HYDRUS uses empirical functions which generate parameters α, n, l (which are empirical coefficients), residual water content (θ_r), saturated water content (θ_s) and saturated hydraulic conductivity (K_s). These parameters are variables to determine soil hydraulic behaviour in unsaturated conditions. The soil hydraulic properties were expressed analytically in HYDRUS with the functions of van Genuchten (1980), Brooks and Corey (1964), as well as a set of modified van Genuchten type functions developed by Vogel and Cislerova (1988).

The solute transport process in HYDRUS can simulate both equilibrium and non-equilibrium conditions. Depending on the type of the process, HYDRUS requires several transport parameters. For equilibrium conditions, longitudinal dispersivity and molecular diffusion coefficient in free water and soil air, if diffusion is considered, are required. For non-equilibrium conditions, dimensionless fraction of adsorption (FRAC) (1 for equilibrium conditions), immobile water content (0 for equilibrium conditions), adsorption isotherm coefficients (*Kd=0, Nu=0, beta=0,* for equilibrium conditions), equilibrium distribution constant between liquid and gaseous phases, and first and zero order rate constants for dissolved and solid phases are required.

HYDRUS-1D requires the meteorological parameters for the estimation of the potential evapotranspiration (by Penman-Monteith, Hargreaves, or Energy Balance methods), and then estimates the actual evapotranspiration based on soil–budget calculations. The estimation of the potential evapotranspiration requires radiation (short wave radiation, cloudiness, emissivity), daily variations of the minimum and maximum temperature and humidity, and wind data. HYDRUS involves a routine called Rosetta developed by Schaap et al (2001) to estimate the soil hydraulic properties from the grain size distribution and bulk density.

3. Experimental research and results

Two unsaturated zone soil profiles were characterized by the soil density, moisture content and hydraulic conductivity. At the Maišiagala radioactive storage facility site undisturbed soil samples were taken to a depth of 380 cm every 20 cm. From a depth of 380 cm to 750 cm disturbed soil samples were collected. The 20 cm soil sample without destroying its structure was divided and placed into 3 equal volume (45.30 cm^3) cylindrical containers. One container with the sample was used for determination of the hydraulic conductivity, 2 for determination of physical–mechanical properties of the soil sample, and the remaining material (destroying its structure) for the extraction of the soil moisture for isotopic analysis.

The unsaturated zone soil profile consists of uniform sand with dry soil density ranging from 1.36 to 1.65 g/cm^3 and natural soil density 1.44–1.68 g/cm^3. Soil hydraulic conductivity under full saturation conditions was determined at the Vilnius University laboratory by the falling head method scheme; when water flows are laminar. The filtration coefficient values vary from 0.9 to 3.9 m/d. Up to 4.5 m depth soil from the profile is air-dry, the degree of water saturation is 0.1 – 0.2 pc. Moisture content ranges from 1 to 7%. From 450 cm soil moisture increases and at a 500 cm depth the soil is saturated with water. Groundwater at the storage area (the first from the ground surface) accumulates in the fine sand deposits.

Observation and analysis of groundwater level changes were performed monthly from 2010 November till 2012 August. Groundwater level monitoring started in October 2010. Groundwater water level at the piezometer during the observation period ranged from 460 cm (April) to 530 cm (January, February) from the surface.

Similar unsaturated zone studies were performed at the Stabatiškė site. For undisturbed structure samples dry soil density ranges from 1.44 g/cm^3 to 2.10 g/cm^3, natural soil density from 1.67 to 2.33 g/cm^3. The filtration coefficient values vary from 0.000013 till 0.4 m/d. For the Stabatiškė soil profile, the moisture content ranges from 5.16 to 22.06 %. There are several layers with lower moisture content at a depth 90–95 cm (6.74%), at a depth 170 – 175 cm (5.16%) and at a depth 190 – 195 cm (5.72%). From 310 cm depth soil is saturated with water.

According to previous studies (Stabatiškės..., 2009), the groundwater level at the piezometer close to the unsaturated zone soil profile and groundwater water sampling place ranged from 215 cm (beginning of April) to 391 cm (end of February).

Stable isotope ratio ($^{18}O/^{16}O$ and $^{2}H/^{1}H$) and tritium (^{3}H) distribution features in the precipitation, unsaturated zone soil moisture and ground water

Global Meteoric Water Line (GMWL) is an equation, which defines the relation between hydrogen and oxygen isotope composition in the worldwide precipitation (Craig, 1961b).

$$\delta^{2}H = 8\delta^{18}O + 10 \qquad (2)$$

The deuterium excess (d–excess), $d = \delta^{2}H - 8 \cdot \delta^{18}O$ (Dansgaard, 1964), reflects the kinetic fractionation effect and is a useful tool for identification the origin of precipitating atmospheric moisture. The average value of modern d–excess for precipitation is 10.

Periodical measurements of ^{3}H, $^{18}O/^{16}O$ and $^{2}H/^{1}H$ ratios in the water samples have been performed. Preliminary relationship between $\delta^{2}H$ and $\delta^{18}O$ for the precipitation (monthly samples of two years 2010 and 2011 from two sampling sites) in East Lithuania was determined in term of the Local Meteoric Water Line (LMWL) (Figure 1):

$$\delta^{2}H = 7.8\delta^{18}O + 7.2 \qquad (3)$$

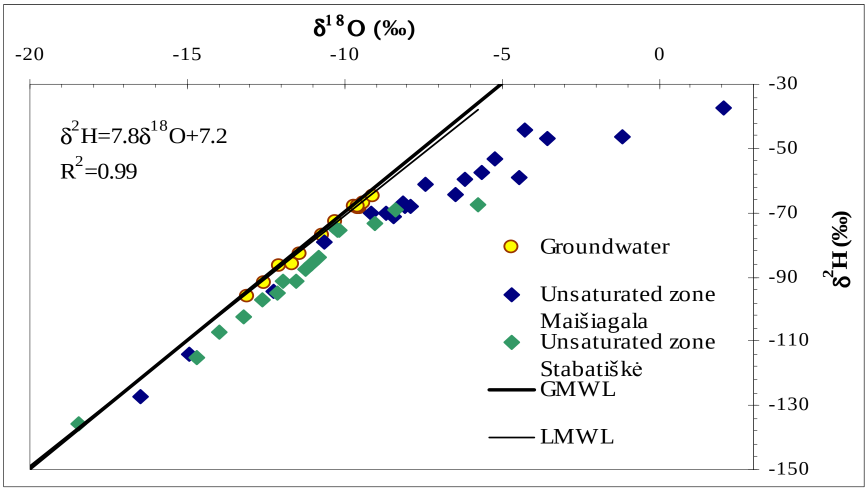


Fig 1. δ^{18}O and δ^{2}H distribution in precipitation, ground water and the unsaturated zone soil moisture

The isotopic composition of precipitation and the local average monthly air temperature are related. The relationship between the isotopic composition (δ^{18}O) of precipitation and local average monthly air temperature, determined in the study areas are as follows:

$$\delta^{18}O=0.31T-12.42 \quad R^2=0.56 \text{ (Vilnius)} \qquad (4)$$

$$\delta^{18}O=0.30T-12.85 \quad R^2=0.64 \text{ (Zarasai)} \qquad (5)$$

During the summer, the isotopic composition of precipitation is less negative compared to the cold period. Monthly precipitation δ^{18}O values range from -20.5‰ (January) to -5.8‰ (September) and δ^{2}H respectively from -154.2‰ to -39.4‰. ^{3}H exhibits seasonal variation in precipitation, as well as stable isotopes, and has a similar annual change trend with maximum values during the warm season. However, long–term observations show that, in addition to seasonal variations, ^{3}H activity has a downward trend (for example, from 11.4 TU average in 1999 to 9.4 TU average in 2012) due to depletion of the ^{3}H originated from thermonuclear explosions. Groundwater stable isotope values were most negative (δ^{18}O = -13.1‰, δ^{2}H = -96.1‰) in March and less negative (δ^{18}O = -9.1‰, δ^{2}H = -65.1‰) in August. Groundwater isotopic data are located on the meteoric water line.

Isotopic composition of the groundwater is close to the annual isotopic composition of precipitation in Lithuania. Due to slow infiltration processes, the observed annual variations in isotopic composition of precipitation in groundwater mostly (except for cases of fast infiltration) almost disappear.

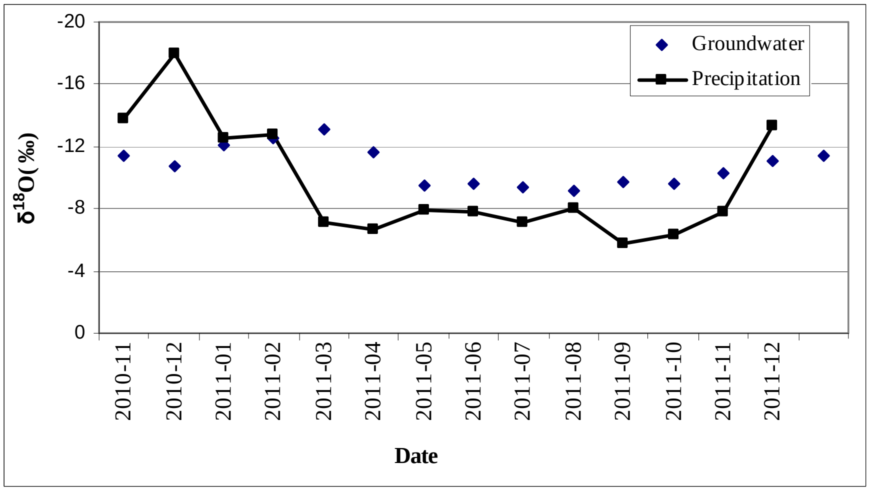


Fig. 2. δ^{18}O change in groundwater (Maišiagala) and precipitation (Vilnius)

The weighed annual mean δ^{18}O and δ^{2}H values for atmospheric precipitation are respectively -9.9‰ and -70‰. The δ^{18}O and δ^{2}H values in the groundwater vary respectively from -12.1 to -9.3 ‰ and from -82 to -70‰. The majority of groundwater samples in diagram (Fig. 2) are situated near the GMWL and LMWL indicating groundwater recharge by modern atmospheric precipitation.

The δ^{18}O and δ^{2}H values of moisture in the Maišiagala unsaturated zone profile vary within wide ranges: from 2.1‰ to -9.1‰ and from -37.5‰ to -70.3‰, respectively. In terms of water isotopic composition, the upper part is much heavier (less negative values) due to enrichment because of evaporation and moisture uptake by plant roots. With the depth of the unsaturated zone profile stable isotope values become more negative.

At the Stabatiškė site unsaturated zone profile, the δ^{18}O and δ^{2}H values of soil moisture ranges from -10.2‰ to -18.4‰, and from -74.6‰ to -135.6‰ respectively.

The ^{3}H activity in the groundwater of the study areas can be related with ^{3}H variation in atmospheric precipitation and in surface water as groundwater recharge sources. The mean annual ^{3}H activity in atmospheric precipitation is about 10 TU.

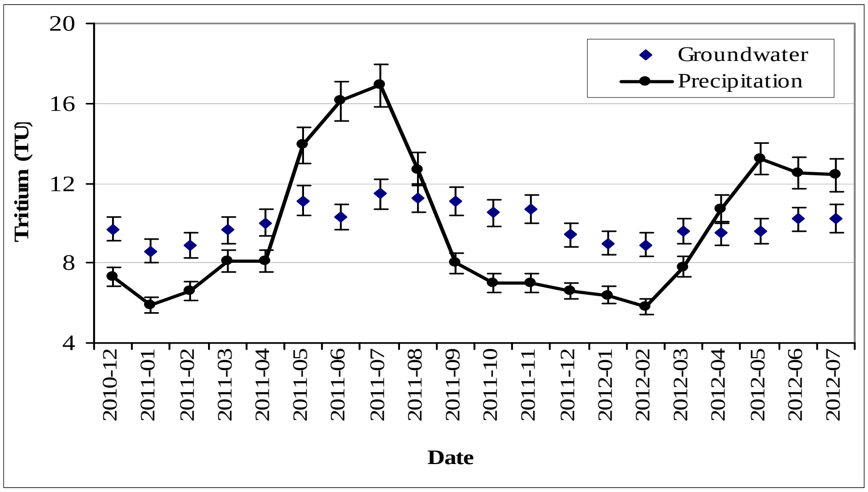


Fig. 3. ^{3}H concentration in groundwater (Maišiagala), and precipitation (Vilnius)

Variations of ^{3}H in the groundwater (the average is approaching 10 TU) are very small compared with precipitation, but the summer period is characterized by slightly higher ^{3}H concentrations (up to 12 TU) (Fig. 3). Generally, the groundwater is characterized by the spring and autumn ^{3}H concentrations in precipitation. The pattern of stable isotopes seasonal variation occurring in the precipitation almost disappear in the unsaturated zone soil moisture and especially in shallow groundwater, but in both sites a slight seasonal peak traces remain, which at the Maišiagala site are a bit more recognizable in comparison with the Stabatiškė site due to the shorter transit time at Maišiagala site.

Performance Assessment of the Near Surface Repository sites

Two nuclear waste disposal sites (Maišiagala, Stabatiškė) were modelled by using unsaturated flow and transport model of HYDRUS-1D (Šimunek et al., 2008). The hydraulic characteristics required for the HYDRUS-1D simulations were estimated based on the analyzed soil properties. The performances of both repositories were analyzed by the similar boundary conditions, expressed by similar scenarios representing low, moderate and high water inputs. The transport of the contaminants to groundwater through unsaturated zone was simulated for an assigned contaminant. In order to estimate the movement of the faster arrival to groundwater, the contaminant was assumed stable (no radioactive decay), and reaction, sorption-desorption and retardation processes were not considered. The effective rainfall input was characterized by different pressure heads on the top of the unsaturated zone. Table 1 summarizes the scenarios. The water input was given in terms of pressure head above the unsaturated zone. Low water input was described by +1 cm pressure head, moderate +10 cm, and high water input conditions were given by +50 cm pressure head.

Table 1. Scenarios of water and solute input

Solute Input (100 unit)	**Water Input (Pressure Head (cm))**		
	Low	**Moderate**	**High**
Instantaneous	1	10	50
Continuous	1	10	50

Since the aim of the study is to identify the risk of the groundwater contamination, in case of any leakage from the waste repositories; the simulations were carried out for a conservative contaminant. Two types of contaminant input functions were assumed in scenarios, instantaneous and continuous. It is assumed that the leakage occurs in 1 day for instantaneous input, and then stops. The leakage does not stop in case of continuous input and continues as simulation period. The leakage concentration is assumed as 100 concentration unit (mass or activity per volume).

The Model Setting

The Maišiagala site. The unsaturated zone at the Maišiagala site is bounded by groundwater table at an average depth of 5 m. The thickness of the unsaturated zone was taken as 5 m. The soil profile in this site is divided into 5 layers by considering the changes in the hydraulic conductivity. The estimated unsaturated soil properties for the Maišiagala site are given in Table 2 for each soil layer.

Table 2. The soil profile layers and their characteristic hydraulic conductivity values

Soil Layer	θ_r **(-)**	θ_s **(-)**	α **(1/cm)**	n **(-)**	K_s **(cm/d)**	l **(-)**	***Density*** **(g/cm^3)**
1	0.00499	0.3187	0.0277	4.1955	230	0.5	1.55
2	0.00386	0.3999	0.045	2.1481	285	0.5	1.48
3	0.0043	0.408	0.0414	2.6113	390	0.5	1.49
4	0.00345	0.3825	0.0476	1.842	176	0.5	1.45
5	0.00463	0.4292	0.0065	1.6758	90	0.5	1.32

The soil profile should be discretized into finite elements. Due to numerical convergence problem, the grid should be denser where the pressure gradient is higher. It is advised to start denser grid at the top of the unsaturated zone where water input creates higher gradient. A total of 751 finite elements was created. The grid size on the top is about 0.01 cm and increased to 1 cm downward. Equal sized grid created convergence problems for the numerical solution. The grid is shown in Fig. 4. The initial water content was defined by the water content measurements in the November of 2010. The initial water content distribution is given in Fig. 5. The date of the measurement is assumed as the beginning of the leakage through the unsaturated zone.

The top and bottom boundary conditions (BC) for the unsaturated zone 1D were defined by the specified head BC. The bottom BC is represented by the water table elevation, whereas the top BC was defined by the height of the water column above the ground elevation representing the water accumulation over the surface of the waste disposal area. The height of the water column is different for each scenario (see Table 1). The bottom boundary is defined by the water table depth and kept constant.

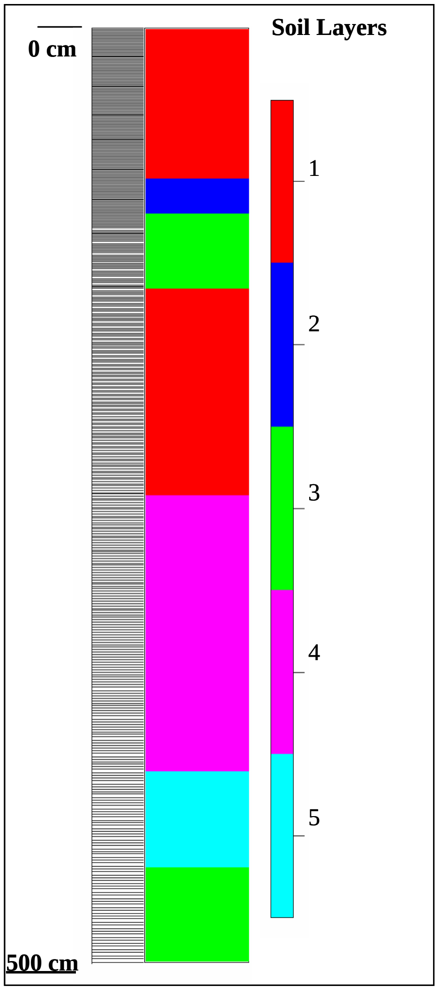


Fig. 4. The distribution of the soil layers and the grid distribution in the unsaturated zone of the Maišiagala site

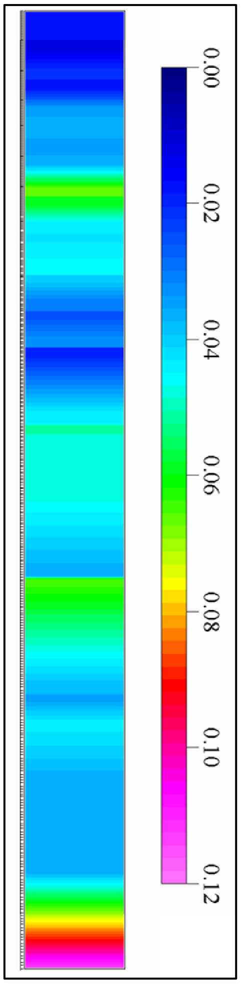


Figure 5 Initial water content distribution based on the measurements in 2010–11–02

The Stabatiškė site. The unsaturated zone at the Stabatiškė site is less permeable when compared with the Maišiagala site. The saturated hydraulic conductivity values are within the range of 1.3×10^{-5} to 0.4 m/d (Table 3). The vertical variability of the hydraulic conductivity indicated the succession of the less permeable soils with more permeable layers. The hydraulic conductivity is lower where the soil is finer. The K value decreases to 5×10^{-3} m/d at a depth of 40 cm, and then increases up to 0.4 m/d at a depth of 190 cm below the surface. Following a thin less permeable layer between 210 to 230 cm depth, K increases up to 0.4 m/d at a depth of 265 – 285 cm. The vertical variability of the K and the existence of the less permeable layers between the high permeable layers cause slower movement of the contaminants at the Stabatiškė than in the Maišiagala site.

According to the grain size distribution and the saturated hydraulic conductivity, the unsaturated zone at the Stabatiškė site is divided into 5 soil layers. The hydraulic characteristics of these layers estimated by the pedotransfer functions are given in Table 3.

Table 3. Hydraulic characteristics of the unsaturated zone at the Stabatiškė site

Soil Layer	θ_r **(-)**	θ_s **(-)**	α **(1/cm)**	n **(-)**	K_s **(cm/d)**	l **(-)**	***Density*** **(g/cm^3)**
1	0.031	0.298	0.0604	1.3735	20	0.5	1.906
2	0.042	0.294	0.0363	1.1853	0.5	0.5	1.538
3	0.073	0.359	0.0106	1.3436	0.12	0.5	1.773
4	0.035	0.326	0.0510	1.5297	40	0.5	1.741
5	0.065	0.439	0.0051	1.6626	0.00013	0.5	1.972

The unsaturated zone at the Stabatiškė site is divided into 961 finite elements (Fig. 6). As in the Maišiagala site, the thickness of the elements is denser where pressure gradients are higher. The grid density is higher where the hydraulic properties change rapidly for numerical convergence. The distribution of the grids and the water content at Stabatiškė site is given in Figs 6 and 7.

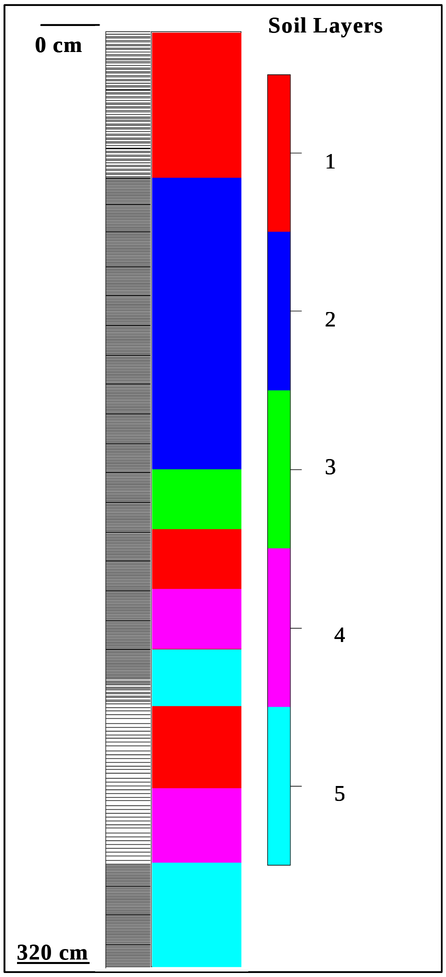


Fig. 6. The distribution of the soil layers and the grid distribution in the unsaturated zone of the Stabatiškė site

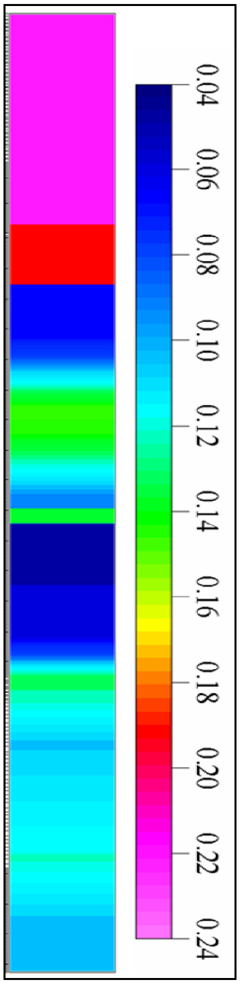


Fig. 7. Initial water content distribution based on the measurements in 2011–06–07

Solute transport

In order to compare the performance of the both sites for nuclear waste disposal, similar pollution scenarios are modelled in both sites with similar input functions. The contaminant could be any matter located in the disposal site. The contaminant is assumed to be conservative and the concentration of the pollutant does not change through chemical reactions or radioactive decay. The transport is modelled only by advection and dispersion. The dispersion coefficient of the medium is not known. For comparison, similar dispersivity coefficients were assigned to both sites. The dispersion is a function of the heterogeneity of the hydraulic properties. Several sensitivity runs were performed to illustrate the role of the dispersion coefficient. Two types of input function were used for the solute transport. The contaminant could enter to the system either by continuous (leakage has not been recognized) or instantaneous (leakage has been recognized and prevented after 1 day) injection. Combined with the low-moderate-high input conditions, 6 different solute transport cases (low-moderate-high water input, and for instantaneous and continuous injection of the contaminant) were simulated for each site.

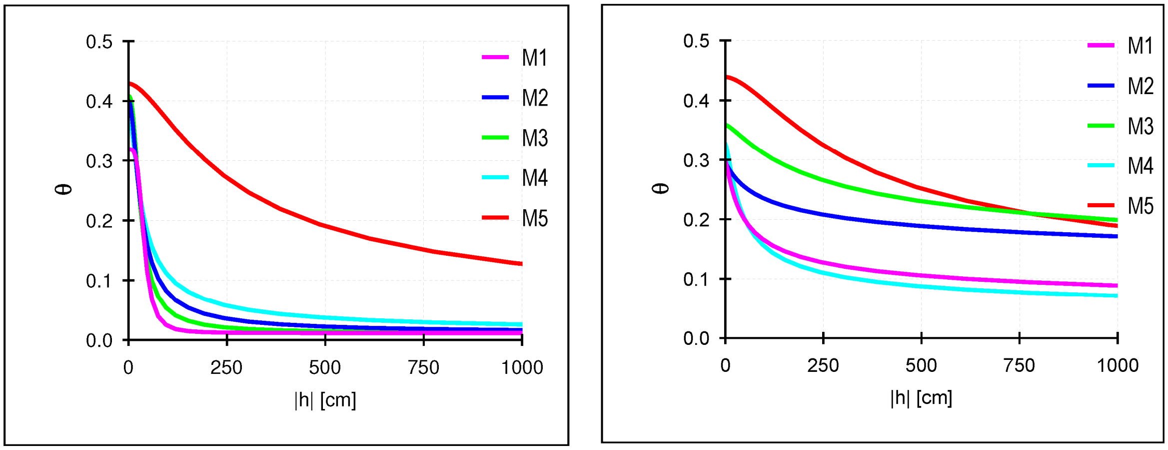
Model Results

Due to great differences in hydraulic properties, the advective movement of the contaminants in the Maišiagala site is much faster than in the Stabatiškė site. Therefore, the time scales of the models are different. The selected simulation time for the Maišiagala Site is 10 days and for the Stabatiškė Site 1000 days.

Soil Properties

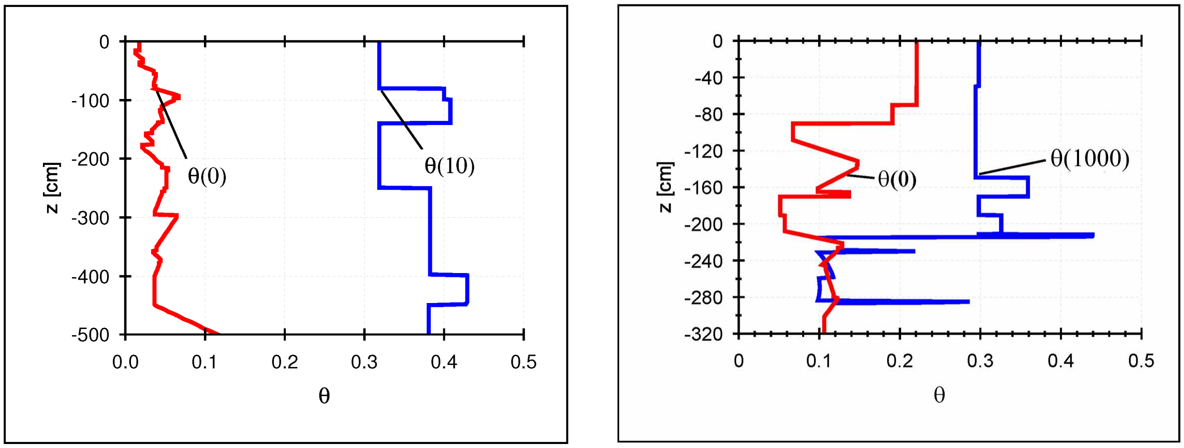
In Fig. 8, the hydraulic properties of both sites in terms of the water content as a function of pressure head in unsaturated zone is compared for 5 soil materials or layers (M1 to M5) at both sites. In Fig. 8, M5 corresponds to the least permeable soil layers at both sites.

In Fig. 9, the water content in the soil profiles of unsaturated zone is compared in both sites for the low input functions (pressure head equals 1 cm). The unsaturated zone at the Maišiagala site becomes saturated in a few days (t=10 days) even at low input, and the water content becomes equal to the specific yield of the soil layers (Table 2). The situation at the Stabatiškė site is different (Table 3). The least permeable soil layer (M5) prevents the downward movement of the water and creates a barrier at 210 cm below the surface. The layers above this horizon become saturated, but water moves very slowly downward, and soil layers below this depth remain unsaturated even after 1000 days.



Maišiagala site Stabatiškė site

Fig. 8. Pressure Head–Water Content Relation at both sites



Maišiagala site Stabatiške site

Fig. 9. Initial water content and simulated water content (t=10 days at the Maišiagala site, t=1000 days at the Stabatiške site)

Maišiagala site. In Fig. 10, the concentration distribution at the bottom of the unsaturated zone (water table) for the continuous contaminant input from the surface is given for the Maišagala Site. The contaminant arrival time is very fast at this site. It is around 14 hours for low and moderate water input conditions, and 12 hours for high input conditions. The 100% of the contaminant arrive in less than 24 hours under all water input conditions. Since the pollutant transport is an advective dominant process due to high permeability of the layers, the influence of the dispersivity is not significant on the concentration time curves.

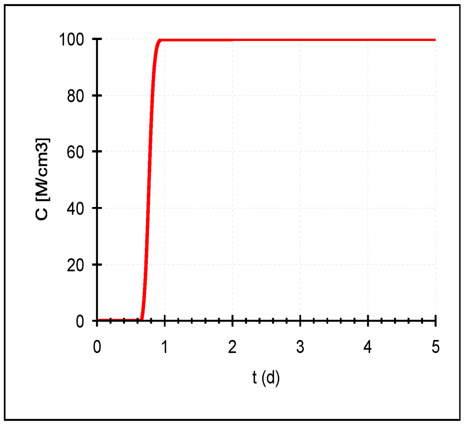
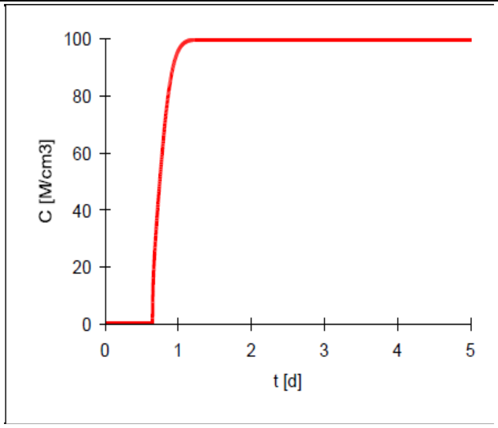
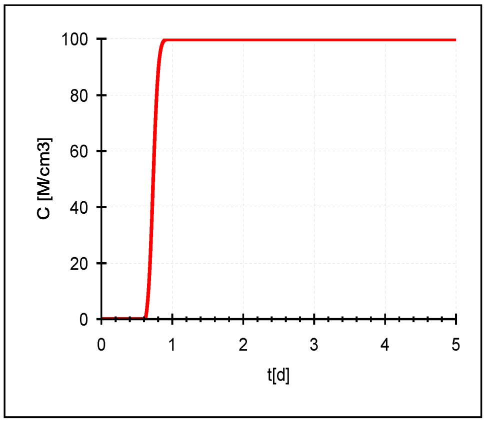
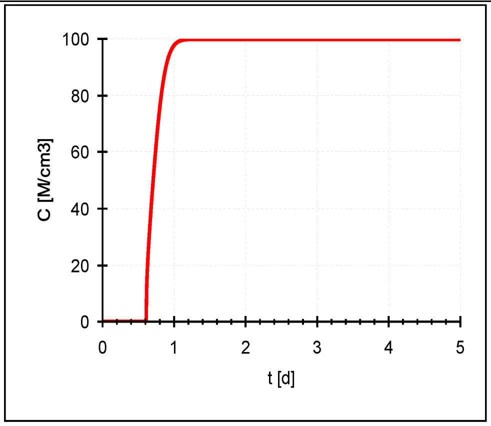
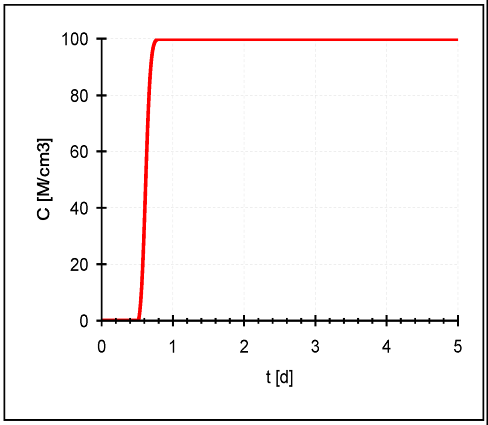
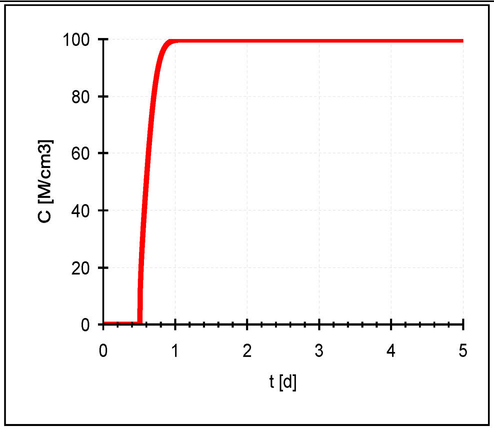
Boundary Head	**Dispersivity α=1 cm**	**Dispersivity α=5 cm**
Low		
Moderate		
High		

Fig. 10. The concentration–time relationship at the bottom of the unsaturated zone at the Mašiagala site for continuous injection for low–moderate–high input functions and different dispersivity (α=1 cm, and α=5 cm) values

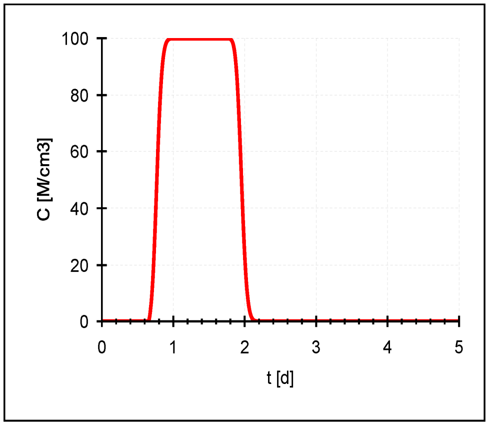
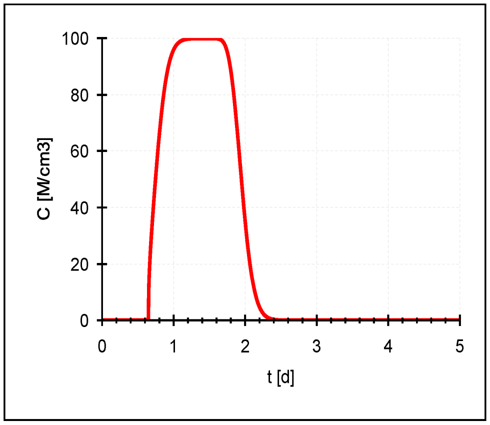
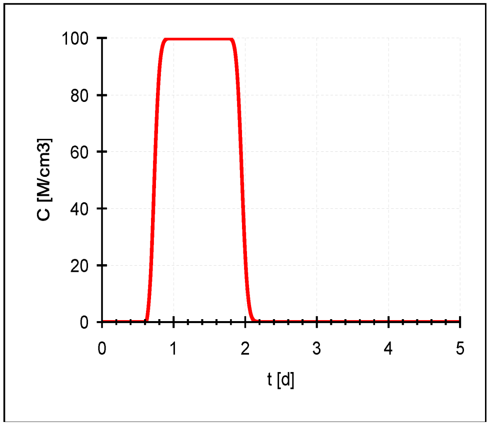
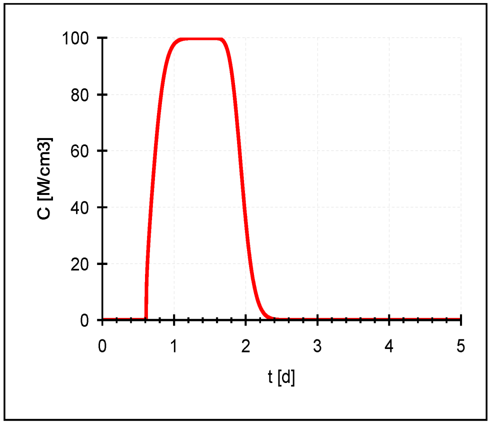
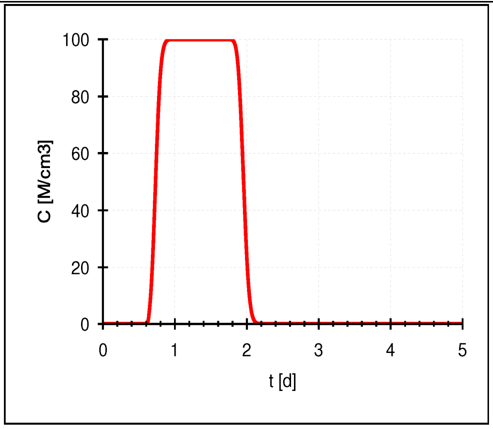
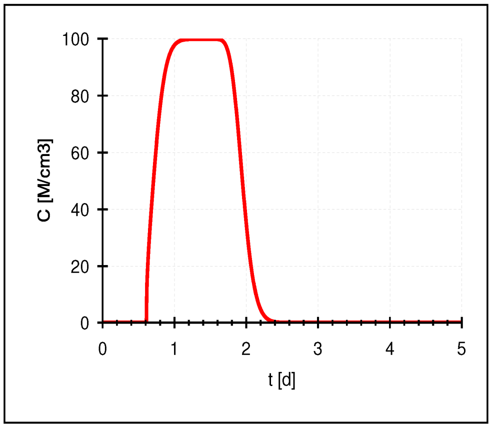
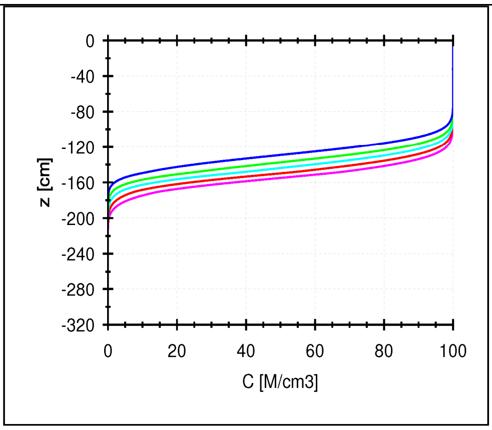
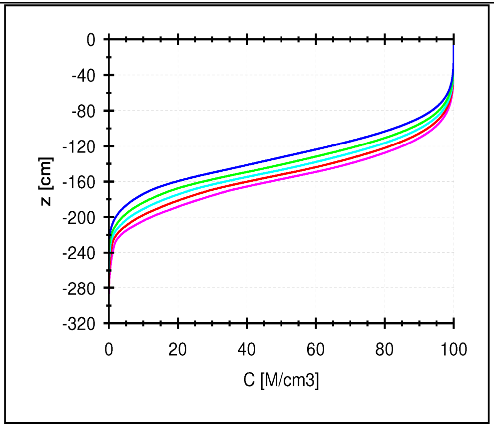
Boundary Head	**Dispersivity α=1 cm**	**Dispersivity α=5 cm**
Low		
Moderate		
High		

Fig. 11. The concentration–time relationship at the bottom of the unsaturated zone at the Maišiagala site for instantaneous injection for low–moderate–high input functions and different dispersivity (α=1 cm, and α=5 cm) values

The concentration–time curves for instantaneous input conditions are given in Fig. 11 for the Maišiagala site. Instantaneous input is simulated by the injection of the contaminant for

1 day and then stopped. Since the water and contaminant transport occurs very rapidly at Maišiagala site, the pollutant arrival time to water table is similar (12 to 14 hours) to the continuous input. The contaminant is completely washed out from the unsaturated zone to the water table in 2 to 2.5 days after the injection.

The Stabatiškė site. The transport of the water and contaminant at the Stabatiškė site is controlled by the existence of the very low permeable layer which is located at depths of 210–230 cm and 285–320 cm. The permeability is relatively higher above these zones, and contaminant arrives to these least permeable zones relatively faster but cannot pass this zone and arrive to the water table in 1000 days of the simulation. Therefore, concentration–depth profiles illustrate the contaminant behaviour better than the concentration–time relationship at the bottom of the unsaturated zone. In Fig. 12, the concentration depth profiles for low–moderate–high input functions and continuous injection are shown for α=1 cm and α=5 cm. The colour of the curves represents the concentration distribution at every 200 days. The contaminant moves relatively faster till the upper least–permeable layer which is located at a depth of 210 to 230 cm, but only very small portion moves to deeper layers. The travel time of the contaminant is much lower than in the Maišiagala site due to lower permeability distribution.

Boundary Head	**Dispersivity α=1 cm**	**Dispersivity α=5 cm**
Low		

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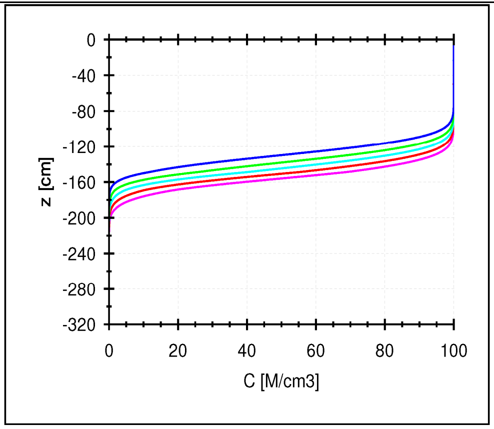
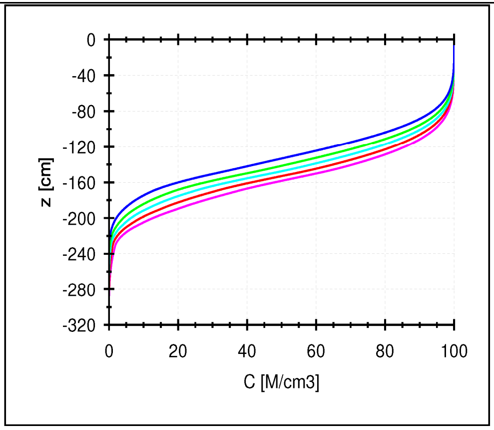
<tr><td>Moderate</td><td>
</td><td>
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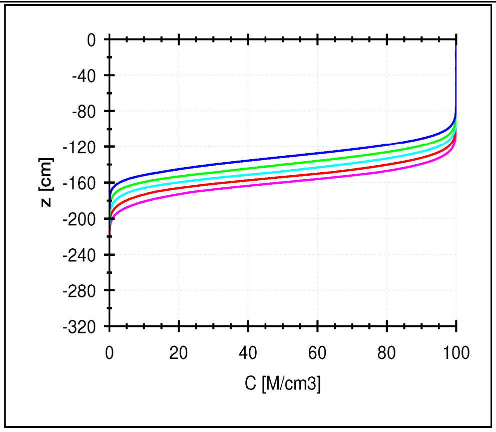
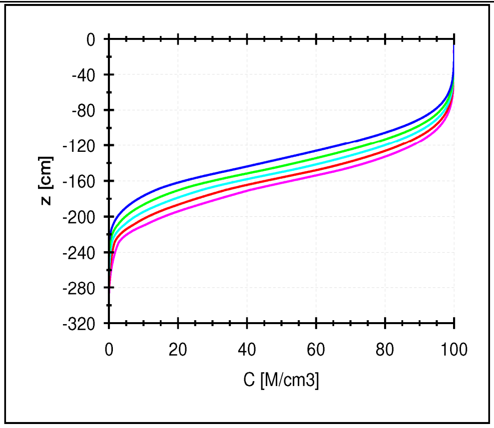
<tr><td>High</td><td>
</td><td>
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Fig. 12. The concentration–depth relations at the Stabatiškė site for continuous injection and low–moderate–high input functions and different dispersivity (α=1 cm, and α=5 cm) values (blue: t=200 d, green: t=400 d, cyan: t=600 d, red: t=800 d, magenta: t=1000 d)

Fig. 13 illustrates the situation at instantaneous injection of the contaminant for 1 day. Similar to continuous injection, the least permeable layer at 210–230 cm acts as a barrier and the contaminant does not move deeper.

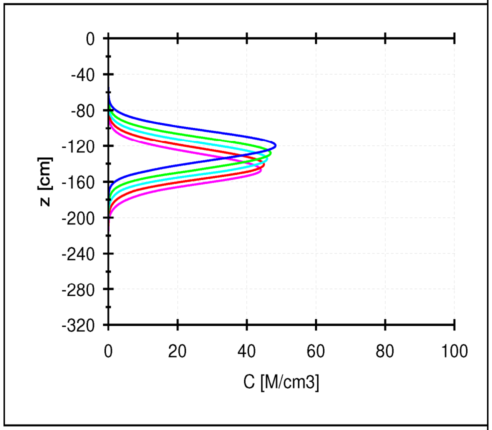
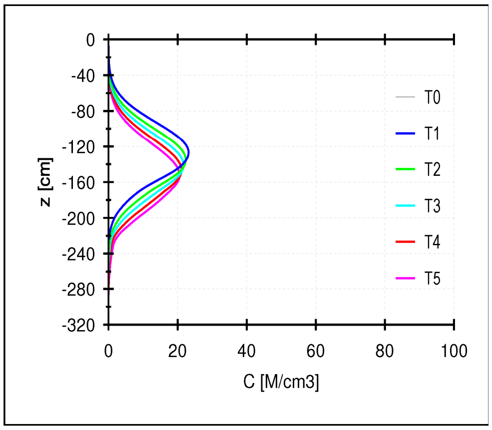
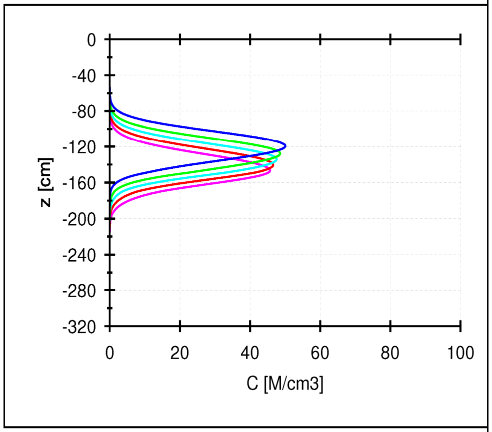
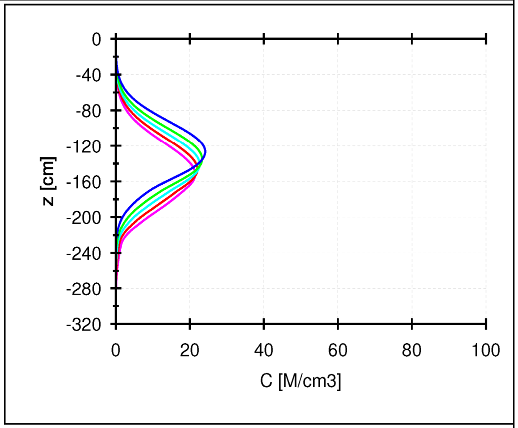
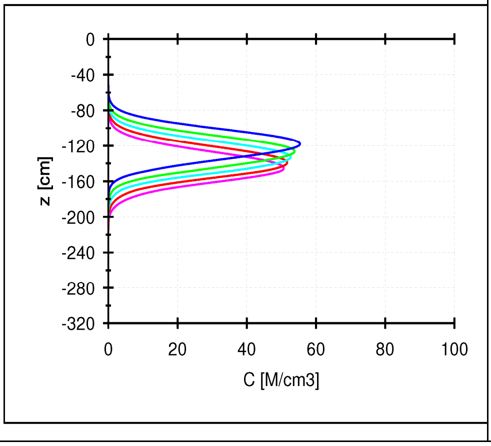
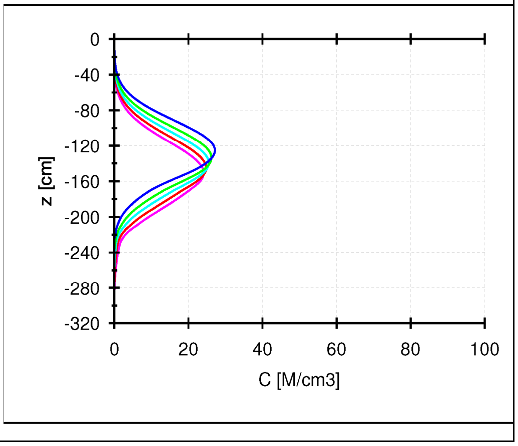
Boundary Head	**Dispersivity α=1 cm**	**Dispersivity α=5 cm**
Low		
Moderate		
High		

Fig. 13. The concentration–depth relations at the Stabatiškė site for instantaneous injection and for low-moderate-high input functions and different dispersivity (α=1 cm, and α=5 cm) values (blue: t=200 d, green: t=400 d, cyan: t=600 d, red: t=800 d, magenta: t=1000 d)

The distribution of concentrations at specific depths (z=50, 100, 200, 250, 300 cm) as a function of time for both continuous and instantaneous injection of the contaminant is illustrated in Fig. 14. The 10% of the contaminant goes to a depth 50 cm in 2 days, to a depth of 100 cm in 11 days, and to 200 cm in 370 days. 10% of the pollutant does not arrive to 250 cm in 1000 days. None of the contaminant arrives to 300 cm, below the least permeable zone in 1000 days. The arrival time to specific depths are similar for both continuous and instantaneous injections, and the role of the water input rate (low–moderate–high) is not significant.

<table>
<tr><th>Boundary Head</th><th>Continuous injection</th><th>Instantaneous injection</th></tr>
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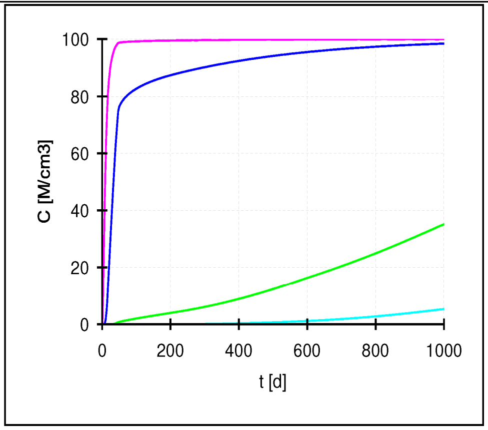

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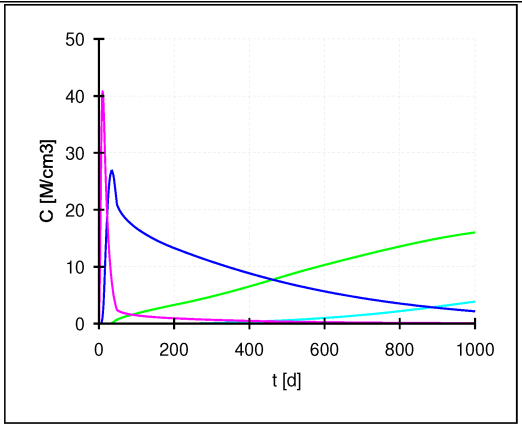

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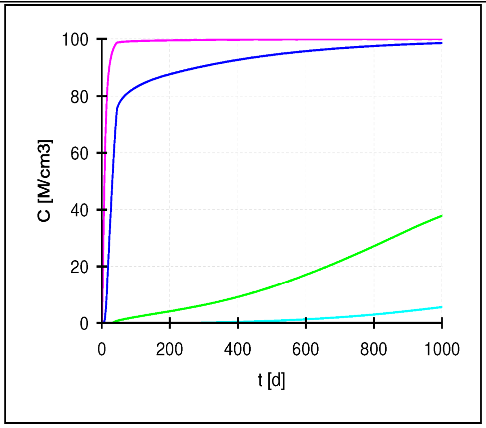

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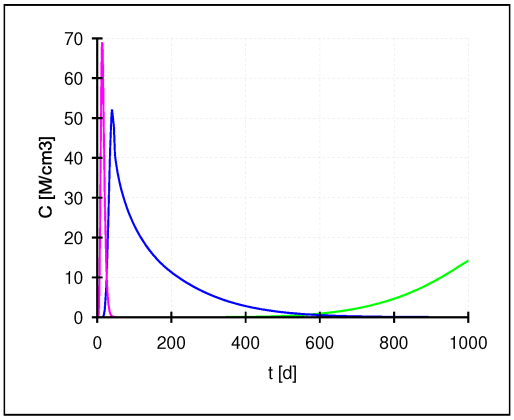

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</table>

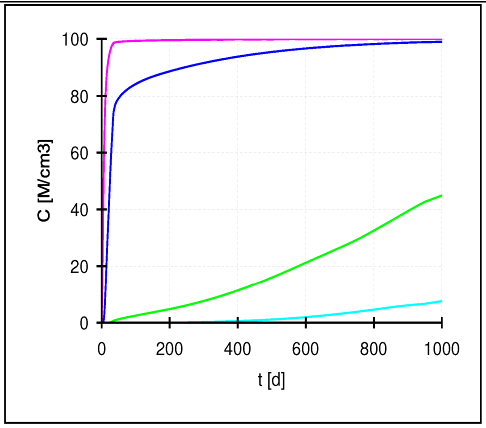
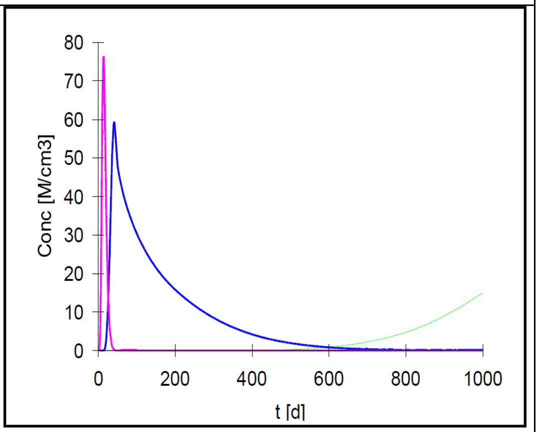
Boundary Head	Continuous injection	Instantaneous injection
High		

Fig. 14. The concentration time curves at z=50 cm (magenta), z=100 cm (blue), z=200 cm (green), z=250 cm (cyan), z=300 cm (red) for continuous and instantaneous injections

Tritium Transport

In order to validate the representativeness of the hydraulic parameters, the model was to estimate the tritium distribution in the unsaturated zone and compared with the measured values in November, 2010. The tritium was inserted into the unsaturated zone by the precipitation. The tritium transport between October, 2009 and the end of December, 2010, was simulated in order to eliminate the influence of the initial conditions on the tritium estimation of November, 2010.

Inputs

Basic inputs of the tritium transport simulation are the tritium input function and meteorological variables (precipitation and potential evapotranspiration). Overland flow was not taken into account. The model is simulated daily. However there is no data available for tritium of the precipitation and the meteorological variables at a daily basis. Since the model requires these inputs at a daily basis, the monthly meteorological values were divided by the number of days of the month with the assumption of uniform values in each day of the month. Monthly tritium values are given same for each day, without dividing by the number of the days, and the tritium input rate (TU/cm^2/d) is calculated by the infiltration rate. The model is simulated by assuming that infiltration and tritium input took place every day. This assumption softens the input function and does not allow simulating the influence of the episodic rain events occurring on some days of the month in greater amounts then on other days. The assumption could be valid for the evapotranspiration but smoothing the precipitation input does not enable to catch the peak or lowest values of tritium.

The tritium input function and the meteorological parameters are given in Fig. 15. The time scale starts from October 1, 2009. The tritium content of the rain varies from 6.2 to 17.7 TU. The maximum potential evapotranspiration was estimated in May, 2010. The rainy period in 2010 occurred between the May and September.

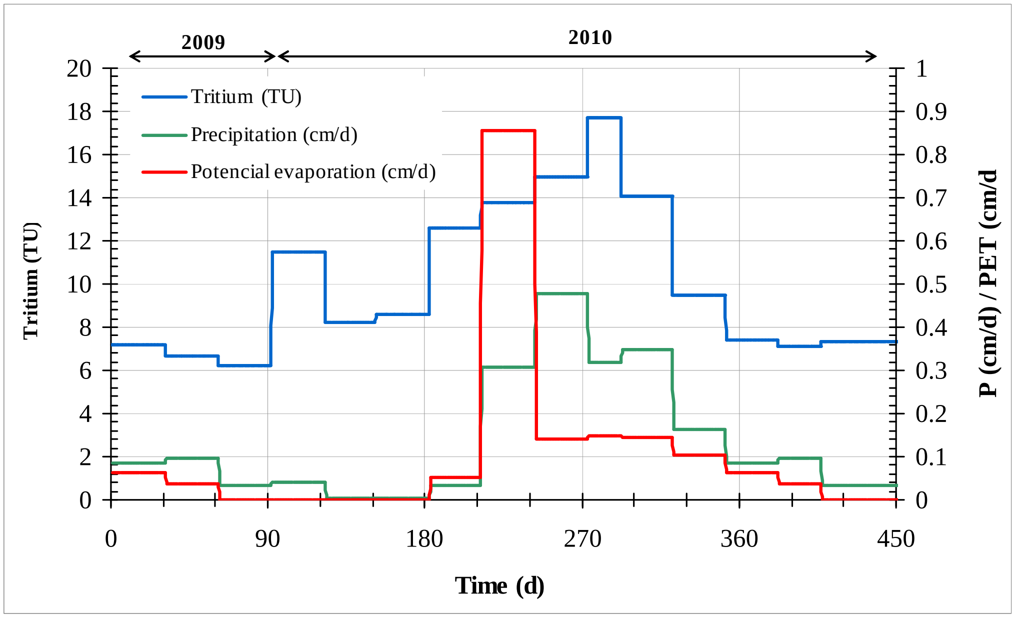


Fig. 15. The tritium input function and the meteorological parameters data

Initial conditions

The initial water content distribution and the initial tritium concentration was created by the model (Fig. 16).

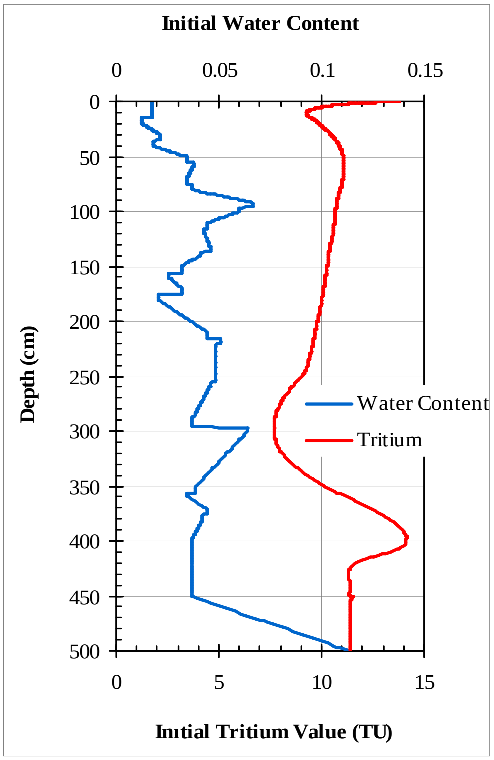


Fig. 16. Initial distributions of the pressure head and tritium in the unsaturated zone given for October 1, 2009

Since the initial conditions have been generated numerically, the estimates of the first months of 2010 could be unrealistic. But the turnover time of the unsaturated system is very fast, and the influences are eliminated until November, 2010.

Boundary conditions

The models used the time-variable BC. The simulation period is 15 months. Each month, a changing value of P and PET (Potential Evaporantion) was given to the model. The bottom of the unsaturated zone is limited with the Water Table which is assumed to be constant throughout the simulation period. Both recharge to the water table and the tritium values reaching the saturated zone are removed from the unsaturated zone, and no accumulation of the water and mass (tritium) occurs due to changing water table level.

The hydraulic parameters are not changed and are identical with the simulations carried out for the performance assessment of the repositories.

Results

As is shown in Fig. 17, the estimated tritium profile is smoother than the measured profile, where the lowest values at depths could not be matched properly.

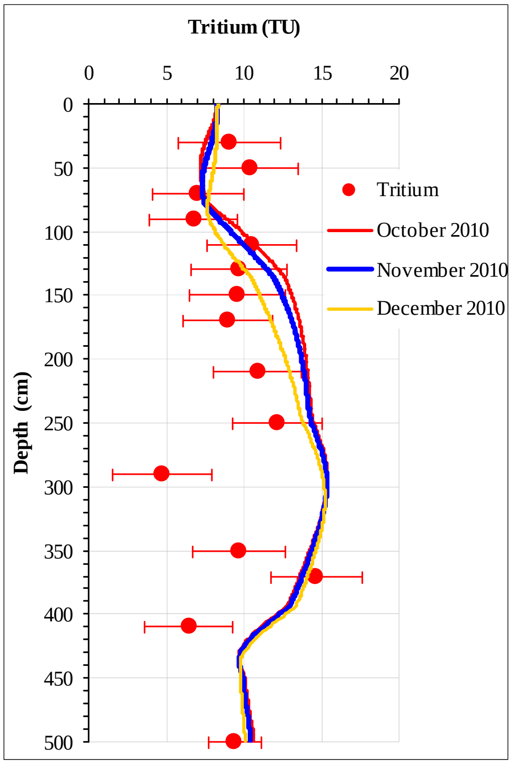


Fig. 17. Comparison of simulated tritium profiles with the measured tritium values in unsaturated zone

The tritium value measured at a depth of 290 cm is considerably lower (4.7 TU) if compared with the tritium of the precipitation observed in 2009 and 2010. This value could be either a result of the low tritium input with precipitation occurring in some days of a month, which is not distinguishable in monthly sum, or due to longer turnover time in considerably less permeable material located at that depth interval. The soil material was examined carefully for permeability measurement and no less permeable material was recognized. In general, the tritium profile fitted well with the observed tritium trend, and the model represents the transport of the water and radionuclides satisfactorily.

Similar to the tritium profile, the water content profile is also smoother due to uniform daily input in each day. The permeability and the flow velocity in the unsaturated zone are very high, and the water content could be closer to the specific retention values in days when no rain occurs. However, monthly rainfall data divided equally in each day, and the estimations are performed with the uniform rain rates for each day.

The model represents the dynamics of the unsaturated zone properly. The uniformity of the daily input in each month should be kept in mind in the evaluation of the smooth changes of the tritium profile and water budget elements.

Conclusions

According to the two years precipitation $\delta^{18}O$ and $\delta^{2}H$ studies, a preliminary local meteoric water line was established, which is for the eastern part of Lithuania expressed as a linear equation ($\delta^{2}H=7.8\times\delta^{18}O+7.2$; $R^{2}=0.9$) and linear relation between the isotopic composition of precipitation and the local average monthly air temperature.

The summer period is characterized by less negative isotopic composition of precipitation if compared with the cold period: monthly precipitation $\delta^{18}O$ values range from -20.5 ‰ (January) to -5.8 ‰ (September) and $\delta^{2}H$, respectively from -154.2 ‰ to -39.4 ‰.

^{3}H concentration fluctuation in groundwater amplitude is very small (the average is approaching 10 TU), compared to precipitation variations, but the summer period is characterized by slightly higher ^{3}H concentrations (up to 12 TU).

At the Maišiagala site $\delta^{18}O$, $\delta^{2}H$ and ^{3}H seasonal peak traces are slightly more contrasting than in the Stabatiškė site, because unsaturated zone moisture transit times are shorter at the Maišiagala site, and the measured hydraulic properties of the unsaturated zone at the Maišiagala site is much higher than in the Stabatiškė site.

There exist a soil layer at the Stabatiškė site located at a depth of 210–230 cm below the surface and it acts as a barrier for water and contaminant transfer. The unsaturated zone above this zone could be saturated due to percolating water. However, this barrier radically prevents the water movement downward. Therefore the contaminant realised at the surface of the Stabatiškė disposal site could reach the water table in a very long time (>35 years) even in case of the continuous injection of the contaminant. The Stabatiškė site is more favourable for nuclear waste disposal in terms of the contaminant movement through the unsaturated zone.

The initial conditions of the water content at both sites have been measured, and the performances of both sites are compared for some scenarios. The transport of the contaminant is simulated for continuous and instantaneous inputs of the contaminant under low, moderate and high water input scenarios.

The measured hydraulic properties of the unsaturated zone for the Maišiagala site are much higher than for the Stabatiškė site. The percolating water and the contaminant within the water move very rapidly due to high permeability layers at the Maišiagala site. The model represents the dynamics of the unsaturated zone properly except the lowest values at depths 280–300 cm which could not be matched properly with the experimental data.

When moisture turnover time in the unsaturated zone is short, ^{3}H transport model is sensitive to ^{3}H input function. In order to improve combination of simulation and experimental results, precise daily ^{3}H input data in precipitation close to the object should be used.

Recommendations

Modelling the radionuclide migration through the unsaturated zone requires precise estimation of the hydraulic conductivity profile and the functional relationship of the hydraulic conductivity and the soil moisture parameters. Several empirical equations (Van Genuchten, Brooks-Corey, etc) used for the unsaturated zone hydraulics requires empirical parameters which could be estimated only by calibration of the numerical model. Therefore, the measurement of the spatial and temporal variation of the water content or pressure head in the unsaturated zone is essential. It is recommended to create a time series of the pressure head measured at several depths under different meteorological conditions (wet and dry seasons). Similarly to the pressure head, the isotope composition of the soil water, groundwater and the precipitation should be sampled and analyzed at different depths and periods. Then the numerical model could be calibrated better and the uncertainty in the estimation of the water and mass fluxes could be reduced.

In the current study, the model has been set only for vertical direction, and the horizontal component of water and mass flux was not considered. The extent and the thickness of the soil layers with the different permeability may not be the same everywhere. Therefore the model should be extended to 2D and a possible horizontal flow components should be taken into account.

The isotope composition of the soil water under natural conditions is controlled by external inputs from precipitation and subject to evaporation. Therefore the temporal series of the isotope composition and the rate of atmospheric inputs (precipitation, evaporation) in the studied areas are essential for the modelling of the water and mass transport under natural conditions. When the model is sufficiently capable to represent the water and mass transport under natural conditions, it can be used for performance testing under different scenarios.

AERACIJOS ZONOS MODELIAI IR JŲ TAIKYMAI RADIOAKTYVIŲJŲ ATLIEKŲ KAPINYNO SAUGOS ANALIZEI

REZIUMĖ

Mokslo ir technologijų pažangos dėka per pastaruosius kelis šimtmečius vis didesne sparta sukuriama daug cheminių ir radioaktyviųjų medžiagų, kurios neretai patenka į aplinką. Daugelis iš šių medžiagų gali patekti į ekosistemų cheminių elementų biogeocheminius ciklus ir kelti pavojų sveikatai, ypač, kai jos įsijungia į maisto grandinę per paviršinį ir požeminį vandenį.

Valstybėse su branduoline energetika ypač aktualūs tampa radioaktyviųjų atliekų tvarkymo saugos klausimai. Sprendžiant šiuos klausimus, didelis dėmesys skiriamas paviršiniams atliekynams (saugykloms ir kapinynams) su gamtiniais ir inžineriniais barjerais. Pastaraisiais dešimtmečiais aeracijos zonos gruntai nagrinėjami kaip pirmasis gamtinis barjeras, gebantis žymiu mastu riboti teršiančių medžiagų sklaidą. Radioaktyviųjų atliekų saugyklose ir kapinynuose esantys radionuklidai ilgainiui per aeracijos zoną gali pasiekti ir užteršti gruntinio vandens sluoksnį bei sukelti pavojų aplinkai ir žmogui.

Lietuvoje anksčiau medicinoje, pramonėje ir moksliniuose tyrimuose susidariusios mažo ir vidutinio aktyvumo radioaktyviosios atliekos šiuo metu laikomos Maišiagalos radioaktyviųjų atliekų saugykloje. Sukauptoms eksploatuojant Ignalinos AE (IAE) ir susidarysiančioms ją išmontuojant trumpaamžėms mažo ir vidutinio aktyvumo radioaktyviosioms atliekoms talpinti bus artimiausiu metu įrengtas kapinynas netoli IAE. Išnagrinėjus Lietuvos teritorijos geologines sąlygas IAE regionas įvertintas kaip labiausiai tinkamas kapinyno įrengimui. Radioaktyviųjų atliekų laidojimas yra paskutinis žingsnis radioaktyviųjų atliekų tvarkymo grandinėje. Tam, kad būtų įvertintas galimas radioaktyviosios taršos poveikis, atliekami tyrimai ir sudaromos įvairių scenarijų radioekologinių padarinių prognozės, modeliuojant radionuklidų migraciją iš radioaktyviųjų atliekų kapinynų bei ją įtakojančius procesus. Prognozuojant atliekose esančių radionuklidų poveikio aplinkai mastą, nagrinėjami radionuklidų pernašos inžineriniuose ir gamtiniuose barjeruose uždaviniai. Drėgmės pernašos procesai aeracijos zonoje netolimoje praeityje

dažnai buvo labai supaprastinami arba apskritai jų buvo nepaisoma, nors aeracijos zonos procesai būdingi ir papildomai įrengiamiems inžinerinių barjerų sluoksniams.

Nagrinėjant vandens judėjimo grunte procesus, įvairių diferencialinių lygčių sprendimui skaitiniai metodai buvo pradėti plačiausiai naudoti tuomet, kai buvo sukurti pakankamai didelių greičių kompiuteriai. Šiuo metu gausu matematinio modeliavimo priemonių, leidžiančių prognozuoti vandens ir jame esančių priemaišų pernašą tarp žemės ir gruntinio vandens paviršių. Tačiau dažnai išlieka modelių kalibravimo eksperimentinių duomenų pagrindu klausimas, ypač tuomet, kai nagrinėjami prognoziniai scenarijai dar tik planuojamiems objektams. Įvairių sprendinių radimas, procesų analizė ir prognozė reikalauja tinkamų priemonių. Kai kurių problemų sprendimui reikia palyginus paprastų analitinių ar pusiau analitinių modelių, kitos problemos reikalauja sudėtingų skaitinių modelių.

Šiame darbe detaliau išnagrinėta ir panaudota kompiuterinė programa HYDRUS, kuri leidžia analizuoti gruntų bei pasirinktų inžinerinių medžiagų savybes, jų kaitą, veikiant krituliams, drėgmės išgaravimui, augalų dangai bei daugeliui kitų aplinkos veiksnių ir procesų. Taip pat galima įvertinti drėgmės bei priemaišų migraciją, esant skirtingo įsotinimo ar pilnai vandeniu prisotintiems gruntams.

Pagrindinis šio darbo tikslas yra charakterizuoti skirtingose hidrogeologinėse sąlygose esančių dviejų branduolinių objektų aikštelių aeracijos zonos gruntus, pateikti aeracijos zonos gruntuose vystančių drėgmės ir priemaišų pernašos procesų charakteristikas ir įvertinti jų ypatumus, taikant kompleksinius eksperimentinius tyrimus ir stebėjimus bei atlikti drėgmės bei priemaišų pernašos skaitinį modeliavimą.

Darbo uždaviniai: parinkti ir optimizuoti aeracijos zonos eksperimentinių tyrimų, stebėjimų ir modeliavimo metodiką; surinkti aeracijos zonos grunto nesuardytos ir suardytos sandaros ėminius; atlikti aeracijos zonos grunto fizikinių-mechaninių savybių ir hidraulinio laidumo tyrimus; atlikti sistemingus gruntinio vandens lygio stebėjimus ir mėnesio kritulių, gruntinio vandens bei aeracijos zonos drėgmės izotopinius (tričio, deguonies-18 ir deuterio) tyrimus; sudaryti aeracijos zonos modelius, pagrindžiant juos *in situ* tyrimų ir laboratorinių eksperimentų rezultatais, ir palyginti saugos požiūriu reikšmingus drėgmės ir priemaišų pernašos aeracijos zonoje ypatumus dviejų branduolinių objektų aikštelėse.

Darbo mokslinis naujumas: pirmą kartą Lietuvoje krituliuose ir aeracijos zonos grunto profilių drėgmėje nustatyti globaliai paplitusio radionuklido tričio (^{3}H) bei vandens molekulės izotopinių traserių (δ^{18}O ir δ^2H) pasiskirstymo ypatumai. Remiantis izotopinių tyrimų duomenimis, sudaryti branduolinių objektų saugos vertinimui svarbūs aeracijos zonos skaitiniai modeliai.

Atlikus eksperimentinius tyrimus ir stebėjimus aeracijos zonos tyrimų aikštelėse ir drėgmės bei priemaišų pernašos skaitinį modeliavimą gautos šios išvados:

Pagal dviejų vietovių dviejų metų trukmės kritulių δ^{18}O ir δ^2H tyrimų duomenis buvo nustatyta preliminari lokali meteorinio vandens linija, kuri rytinei Lietuvos daliai išreiškiama tiesine lygtimi ($\delta^2H=7{,}8\times\delta^{18}O+7{,}2$; $R^2=0{,}9$), ir tiesinis sąryšis tarp kritulių izotopinės sudėties ir jų formavimosi vietovės oro vidutinės mėnesio temperatūros.

Šiltuoju metų laikotarpiu būdingos mažiau neigiamos kritulių izotopinės sudėties vertės palyginus su šaltuoju laikotarpiu: mėnesio kritulių δ^{18}O vertės svyruoja nuo -20,5‰ (sausyje) iki -5,8‰ (rugsėjyje), o δ^2H atitinkamai – nuo -154,2‰ iki -39,4‰.

Lyginant su krituliams būdingoms ^{3}H variacijoms, gruntiniame vandenyje ^{3}H svyravimų amplitudė labai nedidelė (vidurkis artėja prie 10 TV), tačiau vasaros laikotarpiui būdingos šiek tiek didesnės ^{3}H koncentracijos (iki 12 TV) ir gruntiniame vandenyje.

Maišiagalos aikštelėje δ^{18}O, δ^2H ir ^{3}H sezoninių smailių pėdsakai yra šiek tiek kontrastiškesni nei Stabatiškės aikštelėje, kadangi Maišiagalos aikštelės aeracijos zonoje drėgmės tranzito laikas trumpesnis, o hidraulinis laidumas didesnis, lyginant su Stabatiškės aikštele.

Stabatiškės aikštelėje 210–230 cm gylyje yra praktiškai nelaidus sluoksnis, kuris funkcionuoja kaip drėgmės ir priemaišų pernašos barjeras. Aeracijos zona virš šio sluoksnio gali būti periodiškai prisotinta, tačiau šis barjeras labai stabdo priemaišų pernašą žemyn. Šiuo saugos aspektu Stabatiškės aikštelė yra palankesnėse sąlygose nei Maišiagalos aikštelė.

Aeracijos zonos skaitiniame modelyje priėmus hipotetines žemės paviršiaus užtvindymo sąlygas su pastoviu trejopu vandens slėgiu (žemu, vidutiniu ir aukštu), dėl grunto gerokai didesnio laidumo vandeniui ir kitų palankių hidraulinių savybių drėgmės pernaša ir priemaišų advekcija Maišiagalos aikštelės aeracijos zonos profilyje yra daug greitesnė, lyginant su Stabatiškės aikštelės atveju.

^{3}H pernašos Maišiagalos aikštelės aeracijos zonoje modeliavimo rezultatai pakankamai gerai atitinka ^{3}H eksperimentinių matavimų duomenis, išskyrus mažiausią ^{3}H koncentracijos vertę 280–300 cm gylyje. Esant trumpam drėgmės apykaitos laikui aeracijos zonoje, ^{3}H pernašos modelis yra labai jautrus ^{3}H įeities funkcijai. Siekiant geresnio modeliavimo ir eksperimento rezultatų sutapimo, galima būtų naudoti ^{3}H įeities funkcijos paros duomenis, tačiau tam būtini labai detalūs ir tikslūs ^{3}H koncentracijos krituliuose arti tiriamo objekto matavimo rezultatai.

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