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Estimation of hydrogeological parameters of porous media in a radially convergent flow field in Kairėnai polygon, SE Lithuania

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Abstract. In this study, a salt-tracer method applicability in Quaternary aquifer system groundwater was tested. The tracer experiment was performed in Vilnius University Kairėnai polygon for hydrogeological investigations in 2021. In Lithuania, experiments with tracers are not prevalent. Therefore, this work describes the practical use of the tracer for the analysis of the hydrogeological environment, a methodology that enables experiments with salt tracers. After the tracer test, the water flow rate was calculated at the time of the peak concentration of Cl^-, which reached 9.41 m/d. The effective porosity value was calculated manually (0.16) and using TRAC code (0.1389 and 0.1341; normalized for background values). The main results of tracer experiments show that sodium chloride solution is effective as a tracer in the Quaternary aquifer system of Lithuania for actual n_{ef} calculation, where aquifer hydraulic conductivity values are similar to the studied area. Tracer peak analysis performed in this study confirms a possibility of estimating the heterogeneity of aquifer n_{ef} on site.

Keywords: *tracer; peak; cation exchange; effective porosity; TRAC*

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INTRODUCTION

One of the main challenges of hydrogeology is the determination of groundwater parameters (hydraulic conductivity, porosity, dispersion, etc.), water flow rate, and direction. Tracer methods are based on the characterization of groundwater by artificially injected substances: salts, radioactive isotopes, and dyes. Experiments with tracers are useful for understanding groundwater transport and quantifying its parameters in situ without destroying the rock structure and without intrusion into the natural geological environment. The tracer method is used to determine groundwater discharge areas, river water flow rate, groundwater flow in the karst region, soil tests, and possible pollution analysis (Hall *et al*. 1991; Knutsson 1968; Leibundgut, Seibert 2011; Jakimavičiūtė-Maselienė, Cidzikienė 2016). The tracer experiments may provide crucial data parameters required for scientific studies.

Tracer experiments are applicable in Lithuania in many sites where groundwater monitoring is present. Such studies are not limited to well-equipped sites or academic research. Depending on the size and overall consumption of public groundwater extraction sites, usually more than one well is constructed. This enables tracer experiments in these aquifers. Many ecologically sensitive objects (oil refineries, storage facilities, industrial factories, etc.) already have well-developed sets of monitoring wells where tracer tests could be easily conducted. These tests should be specifically designed for each particular site depending on the distance between wells, previous study material, and modelling predictions. Salt tracers could fit some smaller-scale studies and cases where adsorption parameters are required. Dye tracers could be used for research in larger areas – even of regional scale, such as in the karst hydrogeology of northern Lithuania, where the groundwater exchange rate is high. Extensive 3D modelling of Lithuania's Quaternary multilayered aquifer system resulted in calibrated models of groundwater flow and travel trajectories (Mokrik *et al.* 2014; Štuopis *et al*. 2012). These modelling works extended to various attempts for groundwater residence time estimations using tritium, radiocarbon, and computer code simulations. The two main parameters required for such modelling are the hydraulic conductivity and effective porosity of aquifers and semi-permeable layers (Mokrik *et al*. 2014; Štuopis *et al.* 2012). These parameters are usually adjusted in the model calibration phase, using actual data from wells. Hydraulic conductivity could be obtained from the pump test of wells routinely conducted during the approbation of resources (Gregorauskas *et al*. 2008, 2009, 2012). However, effective porosity is often collected from indirect measurements and literature data. The necessity of an actual record of effective porosity measured in situ is crucial for seepage velocity and groundwater residence time calculation.

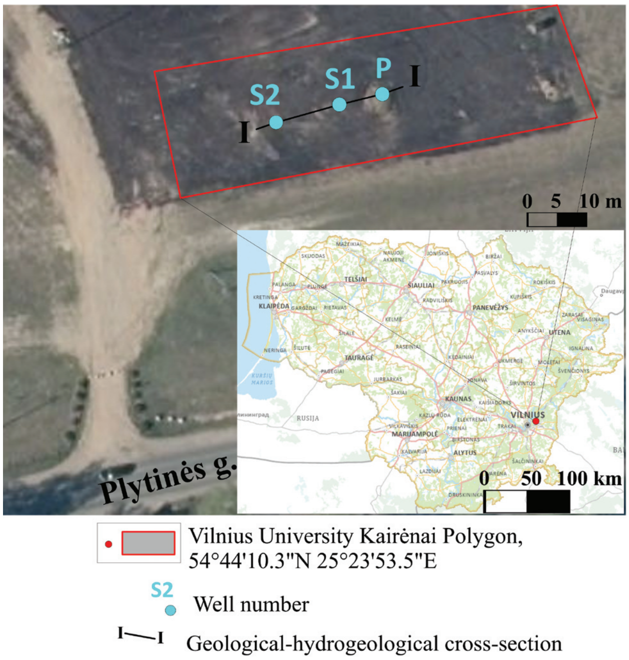

Fig. 1 Location on the Kairėnai polygon specifically designed for hydrodynamic tests in a single aquifer. There are three wells constructed in a row, one of which is equipped with the pump and water extraction infrastructure

Tracer experiment data should act as a proxy for a more accurate modelling of underground environments and routine water management tasks such as resource evaluation and sanitary protection zones determination.

The tracer experiment was performed in Vilnius University Kairėnai polygon (hereinafter, Kairėnai polygon) for hydrogeological investigations in 2021. In Lithuania, experiments with tracers are not prevalent. Therefore, this work describes the practical use of the tracer for the analysis of the hydrogeological environment, a methodology that enables experiments with salt tracers in Lithuania.

GEOLOGICAL SETTING

The Kairėnai polygon is established in the eastern part of Vilnius, Lithuania (coordinates: 54.71825, 25.454672) and is located in the Baltic hills (Fig. 1); the absolute height in the polygon ranges from 131.67 to 131.98 m above sea level.

Quaternary sediments predominate throughout the study area formed during the glacial and interglacial periods (Lithuanian's 1994). However, the upper part of the sediment layer was exarated by glaciers, and there are just fragments of old moraine sediments in this area. The formation of groundwater and hydrogeochemical peculiarities is determined by the lithology of sediment layers, geological conditions, terrain, and precipitation. The lithology of sediments in the study area is heterogenous; there is a slow water exchange through local aquitards (Gribulytė 2013).

Geology

According to the cross-section (Fig. 2), the thickness of Quaternary sediments in the Kairėnai polygon is more than 63 m. The average thickness of the Middle Pleistocene (Žemaitija and Dainava stages) sediments is 44 m and is dominated by grey and brown moraine loam (sandy, silty clay), with gravel and pebbles locally. The Quaternary aquifer complex consists of an unconfined aquifer and three confined aquifers: Grūda (fIIIgr), Žemaitija (aglIIžm), and Dainava (aglIIdn). In the upper part of the cross-section, there occurs an artificial soil with a thickness of 50 cm (Gribulytė 2013). The fluvioglacial fine brown sand with the lenses of various grain size silty sand of the Upper Pleistocene Grūda Stage is lying beneath. Unconfined groundwater is accumulated in these lenses settled on the first continuous aquitard (loam) from the earth's surface and has a good connection with the atmosphere, so the layer is the least protected from possible pollution. Unconfined groundwater occurs at a depth of 6.5–8.5 m, and the total thickness of this layer is 13 m (Gribulytė 2013).

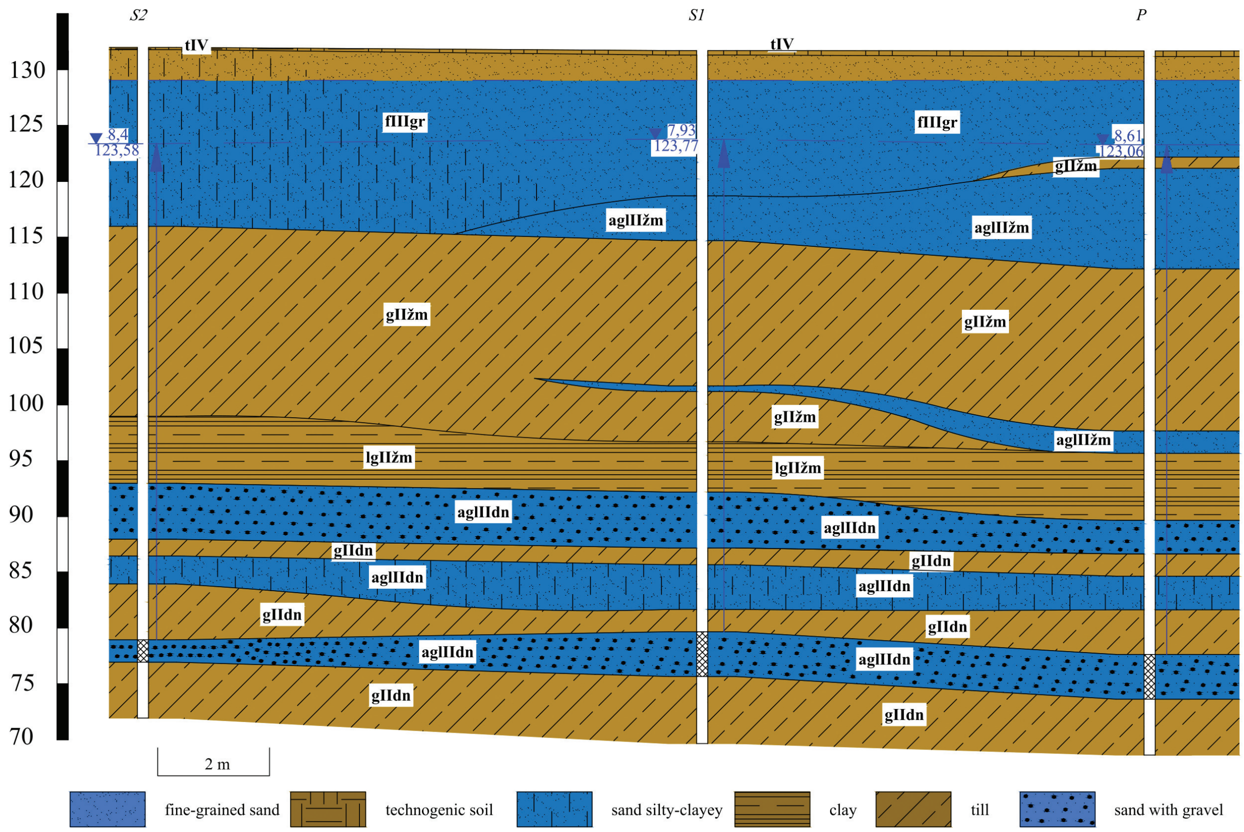

Fig. 2 Geological-hydrogeological cross-section I-I (Fig. 1) of Kairėnai polygon (according to Gribulytė 2013): t IV – technogenic soil; Upper Pleistocene aquifer: fIIIgr – Grūda fluvioglacial; Middle Pleistocene aquifers: aglIIžm – Žemaitija aquaglacial, aglIIdn – Dainava aquaglacial; Middle Pleistocene aquitards: gIIžm – Žemaitija glacial, lgIIžm – Žemaitija limnoglacial, gIIdn – Dainava glacial; blue line – static water level indicated by blue number

Hydrogeology

The total thickness of the Middle Pleistocene aquifer is approximately 29 m. The layer of silty sand of the Middle Pleistocene Žemaitija Stage overlays the test aquifer at a depth of 10.5 m from the earth's surface. Thus, the Kairėnai polygon is in a heterogeneous hydrogeological-geological system with six aquitards and six aquifers that are hydraulically connected horizontally and vertically (Gribulytė 2013).

The gray moraine loam (sandy-silty clay) with gravel and pebbles of the Žemaitija Stage occurs at a depth of 19.5 to 36 m; its bed contains 2 m thick aquaglacial fine clay sand. At a 42– 45 m depth, the Žemaitija Stage is replaced by the aquatic Dainava Stage consisting of aquaglacial various gravelly gray sand, which accumulates confined groundwater. This layer is bounded by two low-permeable layers of limnoglacial Žemaitija Stage gray clay and Dainava Stage glacial gray moraine loam (sandy-silty clay). Beneath, the loam (sandy-silty clay) is replaced by 4 m thick aquaglacial Dainava Stage gray fine silty sand with gravel and pebbles. Below this layer, at a depth of 54–58 m, gray sand with gravel of the Middle Pleistocene Dainava Stage is lying. The hydrogeological parameters were determined during test pumping: water yield – 2.50 l/s, specific yield – 0.089, and water declension – 28 m from the earth's surface. This confined aquifer is bounded by an average 5 m thick gray moraine loam (sandy-silty clay), which lies above it, and another aquitard below, which consists of the gray moraine loam of the Dainava Stage (sandy-silty clay). The total groundwater flow moves north towards the Veržuva rivulet, which is discharged into the Vilnelė rivulet (Fig. 3) (Gribulytė 2013).

Groundwater composition

An analysis of the hydrogeochemical composition of aquifer groundwater at a depth of 54–58 m was performed in 2012. Water samples were taken from the pumping well (well P in Fig. 1). Water analysis shows that the water is neutral (pH is 7.4), hard (total hardness is 7.01 mg-eq/l), and of low total dissolved solid content (519 mg/l). The water is calcium-magnesium bicarbonate, mainly bicarbonate (378 mg/l) and chloride (3.11 mg/l), while the cations are dominated by calcium (98.92 mg/l) and magnesium (25.17 mg/l). The concentrations of sulphates and potassium ions are low (SO_4^{2-} – 0.8 mg/l; K^+ – 2.35 mg/l). Ammonium ions do not exceed the maximum permissible level (0.5 mg/L) (Gribulytė 2013).

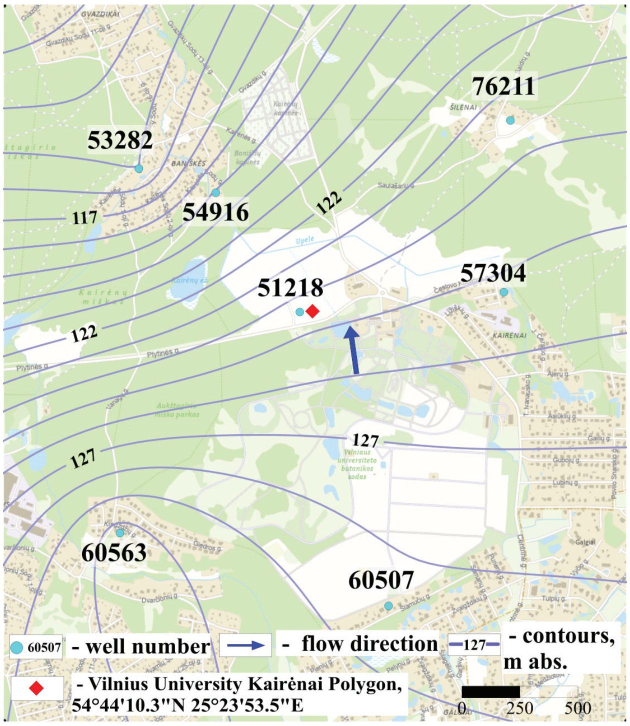

Fig. 3 Hydrodynamic scheme of the Dainava aquifer. Red dot indicates the Kairėnai polygon

METHODS

The tracer experiment was performed in the Kairėnai polygon in 2021. The data from the previous investigations performed during the Kairėnai polygon installation (Gribulytė 2013) and during tracer experiments using fluorescent dyes (Mažonas 2020) were also used. To conduct the field tracer test, three well settings were used (Fig. 1). The well labelled with P was the pumping well, S1 was the tracer input well, and S2 was the water table observation well. The three wells were in a line; the injection well was 8 m away from the pumping well. The thickness of the aquifer was about 4 m. The pumping of the well was started before salt injection. The pumping rate was constant throughout the whole experiment. The salt tracer was injected into the S1 well after the steady-state was reached using a submersible pump. Groundwater was pumped at a rate of 0.0014 m^3/s at well P, and when groundwater level became stable (steady-state), the tracer (50 l NaCl with the concentration of 100 g/l) was injected into the aquifer at the injection well (S1). Before injecting the tracer into the aquifer, the background value of the tracer in groundwater was determined: SEL (µS/cm) – 593, concentrations of Na^+ and Cl^- (mg/L) – 9.3 and 2.9, respectively. After the tracer was injected into the aquifer, water samples were collected from the pumping well every 5–30 minutes; the total duration of groundwater pumping was 1475 min. (≅ 25 h). The frequency of water sampling depends on the specific electrical conductivity value (SEL); the highest frequency of 5–10 min was chosen when specific electrical conductivity was getting higher.

The drawdown values at the end of the experiment were: pumping well –24.4 m (99.28 m a. s. l.); injection well – 11.50 m (112.27 m a. s. l.); investigation well –11.71m (111.35 m a. s. l.).

According to the experiment results with the tracer, the groundwater flow rate and the effective porosity of the soil were evaluated. The velocity of mass transport was calculated:

$$u = \frac{L}{t_{max}}, \tag{1}$$

L – distance between injection and observation wells, m; t_{max} – time of transport of peak tracer concentration, s (Davis *et al.* 1985).

The effective porosity can be calculated by the transfer rate of the tracer (Hall *et al.* 1991; Stephens *et al.* 1999):

$$n_{ef} = \frac{k \times I}{u} = \frac{v}{u}, \tag{2}$$

k – hydraulic conductivity, m/d; I – hydraulic gradient; u – velocity of mass transport (seepage velocity), m/d; v – Darcy velocity, m/d.

The results were analysed using computer tracer test interpretation for porous environments code TRAC developed by the French geological survey (BRGM) (https://www.brgm.fr/en/software/trac-computer-assisted-tracer-test-interpretation-porous-environments). TRAC is based on analytical solutions and can simulate and design tracer tests or interpret results. The interpretation of the tracer test results in the Kairėnai polygon was performed using a brief injection of mass in radial convergent flow induced by a continuous pumping well method (Manuel 2012). The TRAC analytical solutions are given by (Sauty 1978):

$$C\,(x,t) = \frac{M_0 r}{2Q_p t^{\frac{3}{2}}\sqrt{\pi \alpha_L u}} \exp\left(-\frac{(r-ut)^2}{4D_L t}\right)\exp(-\lambda t), \tag{3}$$

C – concentration of the tracer at point (x,y) and time (t), kg/m^3; M_0 – mass of the injected tracer, kg; Q_p – pumping rate, m^3/s; α_L – longitudinal dispersivity, m; u – pore velocity/ m/s; r – radial distance injection-restitution, m; t – time, s; D_L – longitudinal dispersion, m^2/s; λ – decay constant, 1/s; x – distance between measurement and injection points regarding x-axis, m.

The values of injected tracers were interpreted and optimized using computer code TRAC. The interpretation is determining the parameters of the aquifer by calibration. This is done by selecting one of the available analytical solutions and, from a set of given parameters and a range of possible values, the software search for an optimized best fit. Computer code TRAC lets define any quantity of parameters to optimize (Gutierrez *et al*. 2013).

RESULTS AND DISCUSSION

Effective porosity calculation

The field tracer test was conducted in the Kairėnai polygon for about 25 hours, and a total of 110 water samples were collected from the observation well. The specific electrical conductivity value increase was considered to be a result of tracer salt concentration elevation. The variations of tracer's (Cl^-) concentration with time are shown in Figure 4. It's seen that tracer's concentration began to increase 750 minutes after the start of the field test, and after about 1225 minutes in the observation well, the specific electrical conductivity and the Cl^- concentration reached peak values, respectively, 668 µS/cm and 24.24 mg/L, then gradually decreased back to the background level.

The hydraulic conductivity of the aquifer in this site was estimated to be 0.96 m/d (Gribulytė 2013). The hydraulic gradient was calculated for the steady-state and assumed for the whole duration of the experiment and calculations. Darcy velocity was calculated using new experimental data and reached 1.6 m/d, and seepage velocity was 9.4 m/d (Eq. 1). The resulting effective porosity was 0.16 (Eq. 2). The results were also analysed using computer code TRAC (Fig. 4, Table 1).

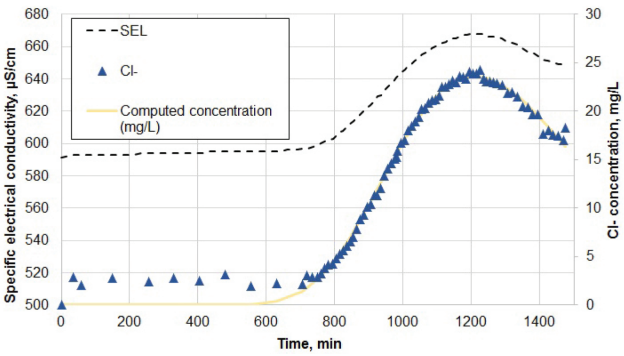

Fig. 4 Distribution of tracers (SEL and Cl^-) and TRAC-computed Cl^- concentration variations with time

Table 1 The parameters of the investigated aquifer

	Measured	Experimental 2021	Experimental 2021, normalized
Mass, kg	–	4.006	2.39
Longitudinal dispersivity, m	–	0.1532	0.1498
Kinematic/effective porosity	0.16	0.1389	0.1341
Radial distance, m	–	7.282	7.314
Average filtration velocity, m/s	1.77e-5	9.15e-5	9.8e-5
Aquifer width, m*	8	7.955	7.955
Pumping flow, m^3/s	1.429e-3	2.354e-3	2.254e-3

* – distance between pumping and investigation well.

The hydraulic conductivity values were calculated according to the data obtained during the installation of the wells. It was done in several methods. In this work, the hydraulic conductivity values calculated through chronological semi-logarithmic graph analysis were used. Hydraulic conductivity in well P was 0.96 m/d (Gribulytė 2013).

After the tracer test, the water flow rate was calculated at the peak concentration of Cl^- and reached 9.41 m/d. According to the time of Cl^- first appearance (after elimination of background values) in the observed well, the water flow rate was 15.38 m/d.

The obtained effective porosity values were: manual calculation – 0.16 and using TRAC code – 0.1389 and 0.1341 (Table 1). Previous studies show the modelled effective porosity to vary in the range of 0.1–0.3 in the aqIIdn aquifer (Mokrik *et al.* 2014; Štuopis *et al.* 2012). Since the effective porosity value of 0.01 is extremely low and natural soils do not have such effective porosity values, it can be considered that the only accurate value of effective porosity is 0.16 and the hydraulic conductivity value of 0.96 m/d is correct. Such low values of n_{ef} would result in a very low yield of the aquifer and cannot be attributed to it but rather to semi-permeable layers. The effective porosity value of 0.16 is typical of clayey sand with effective porosity ranging from 0.15 to 0.37 or of gravel/silty sandy gravel with effective porosity ranging from 0.15 to 0.2 (https://structx.com/Soil_Properties_006.html).

During the construction of the Kairėnai polygon, the lithological composition of the aquifers was analyzed. It is known that the aquifer consists of silty sand with gravel and pebbles, so it can be confirmed that the lithology of the aqueous layer is gravel/silty sandy gravel after measurements of hydrogeological parameters of the tracer test. The hydraulic conductivity of the aquifer is in line with the values found in the literature for analogous lithological composition (Domenico, Schwartz 1990).

Peak analysis

The time required for a tracer to travel the distance may suggest some insights into the aquifer hydraulic properties heterogeneity along the flow path. Tracer signal analysis may be conducted using the peak analysis (Samalavičius, Mokrik 2016). An example of tritium peak sections into a couple of possible arrival times may be applied as an analogy to the tracer. The peak analysis constitutes two reference points (Fig. 4): the beginning of the peak (BP) and the peak maximum (PM). In cases when the background values of the tracer content are reached after the injection, the peak endpoint (PE) may also be deduced. In our study, extrapolation is required for a theoretical PE to obtain. A usual tracer analysis is based on the peak maximum, considering other parameters of mass transport such as advection, dispersivity, diffusion, and retardation. Using the peak analysis method, three seepage velocity values could be calculated.

In our study, different times required to reach each peak point were 1225 min (PM), 750 min (BP), and 1900 min (PE) (Fig. 5). According to these times, variation of a theoretical n_{ef} in the tested section of the aquifer could be established as follows: 0.10 for BP, 0.16 for PM, and 0.26 for PE. The heterogenic hydraulic properties of the aquifer matrix, diffusion, and dispersion predetermine the shape of the peak as a time difference between elements' BP, PM, and PE. This approach may help evaluate a possible n_{ef} variation in the section of the aquifer where the tracer was flowing. However, 0.16 for PM should be considered the average n_{ef} value of this aquifer section, which is entirely acceptable in many cases. The calculation of n_{ef} is based on chloride, which is an inert conservative species. Chloride does not participate in the aquifer matrix-groundwater system's chemical reactions to significantly alter its concentration. However, the NaCl tracer released underground may alternatively be used to analyze sodium peak.

Cation exchange

In Figure 5, sodium and chloride content is corrected by subtracting background values, 2.5 and 7.2 mg/L, accordingly. The signal represents the content that originates exclusively from the tracer material. Both peaks should coincide because NaCl provides equal parts of sodium and chloride equivalents. However, sodium content is significantly lower (almost twice as expected) compared to chloride. An additional factor must be accounted for to explain this phenomenon.

Contrary to chloride, sodium may participate in cation exchange (CE) between dissolved components and the aquifer-bearing mineral matrix (Chapelle, Knobel 1983; Toran, Saunders 1999). An example of this process occurs in the freshwater aquifers, where seawater intrusion exists (Walraevens, Camp 2004; Walraevens *et al.* 2001). The interaction of seawater (rich in sodium) with a Ca-dominant matrix of the aquifer results in the absorption of Na^+ and release of Ca^{2+} into the solution, reaction equation (Appelo, Postma 1993; Appelo 1992):

$$Na^+ + \frac{1}{2}Ca^{2+}X \rightarrow \frac{1}{2}Ca^{2+} + Na^+X. \qquad (4)$$

An analogical situation occurs when NaCl tracer is introduced into a freshwater Quaternary aquifer. The initial chemical groundwater type is Ca-Mg-HCO_3 which originates from the carbonate mineral dissolution. This type of groundwater indicates that calcium ions dominate aquifer minerals (exchanger). The resulting reaction leads to a decrease in sodium content and an equivalent increase in calcium. Therefore, significant differences

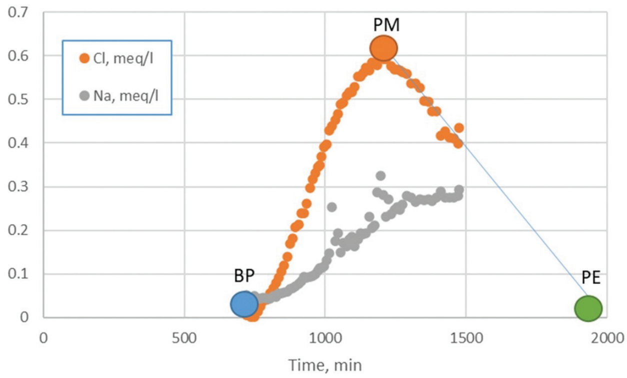

Fig. 5 Chloride and sodium (meq/l) content diagram. The content is adjusted for the background content of sodium and chloride to represent the tracer portion of the components. Peak analysis abbreviations: beginning of the peak (BP), peak maximum (PM), peak endpoint (PE)

between chloride and sodium peak maximum occur. Due to their high surface area, the aquifer matrix clay particles are usually the most important cation exchange agent. Organic matter, oxides, and hydroxides present in aquifer solid matter also increase the CE capacity (Appelo, Postma 1993). The sodium peak (Fig. 5) appears to be stabilizing in the time interval of 1300–1500 min, contrary to the decrease of chloride.

This observation may be due to the saturation of the aquifer matrix with sodium when an opposite reaction starts – the release of Na^+ to the solution. The sodium content may be at this point until a new equilibrium is reached. The data, however, is insufficient to approve the reverse reaction reliably.

CONCLUSIONS

This work describes the practical use of the tracer for the analysis of the hydrogeological environment and a methodology that enables experiments with salt tracers in Lithuania. The first investigations of the hydrogeological parameters were fulfilled during the installation of the Kairėnai polygon wells, and the hydraulic conductivity values were calculated. The results of chronological semi-logarithmic graph analysis were used for the planning and interpreting of tracer experiments with salt (Cl^-). The main results of tracer experiments show that sodium chloride solution is effective as a tracer in the Quaternary aquifer system of Lithuania for actual n_{ef} calculation. Chloride and SEL are reliable parameters to analyze tracer migration as well. Sodium species are sensitive to cation exchange; therefore, it should not be used as an analytical element to calculate hydraulic parameters. Tracer peak analysis performed in this study may be used for estimating aquifer n_{ef} heterogeneity on site. However, a record of actual n_{ef} is required for a more accurate evaluation of groundwater resources, modelling, and contamination prevention assessments. Multiple tracer experiment data should support peak analysis effectiveness. Cation exchange should be studied and noticed in other sites and aquifers of the Quaternary system to evaluate the reaction rate and exchange capacity of minerals in situ. Salt tracers could be practically used in Lithuania as a routine procedure because all the necessary infrastructure already exists in many cases.

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