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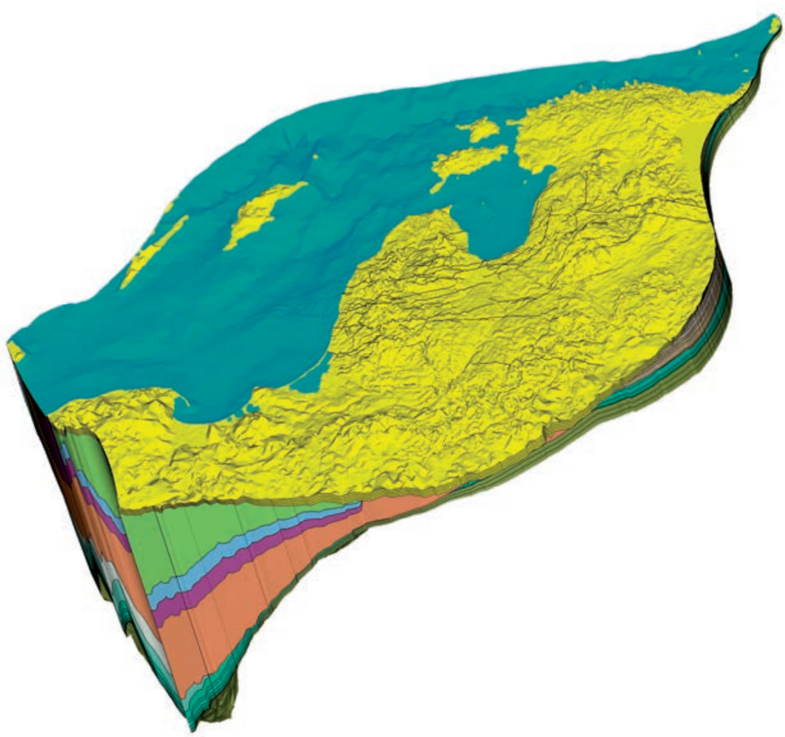
HIGHLIGHTS OF GROUNDWATER RESEARCH IN THE BALTIC ARTESIAN BASIN



Highlights of groundwater research in the Baltic Artesian Basin

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Preface

The Baltic Artesian Basin (BAB) is found at the western corner of the East-European platform. In the east it is delimited from the much larger Moscow basin by diverging groundwater flow patterns and anticline structures. The underlying basement reaches the surface along the northern border of the sedimentary basin; its western boundary is determined by the Teisseyre – Tornquist fault zone, whilst the southern edge – by the Byelorussian – Masurian anticline. Geographically the BAB roughly corresponds to the territories of Estonia, Latvia and Lithuania, the Kaliningrad region of the Russian Federation and the central part of the Baltic Sea reaching the island of Gotland, with its outskirts in northern Poland, north-western Byelorussia and the very west of the mainland of the Russian Federation.

A detailed introduction about the geological evolution of the Baltic sedimentary basin is given in this book, followed by multidisciplinary highlights of the research evolving around groundwater issues.

The compendium emerged as a result of studies performed in a multidisciplinary group brought together within the framework of a three year long project "*Establishment of interdisciplinary scientist group and modelling system for groundwater research*[1]" which was launched in 2009. A group of PhD students, recent PhD graduates and foreign scientists in the field of geology (Faculty of Geography and Earth Science of the University of Latvia) teamed up with an experienced group of modellers (Faculty of Physics and Mathematics of the University of Latvia) and engineers (Faculty of Rural Engineering, Latvian University of Agriculture) to establish a mathematical model of the Baltic Artesian Basin. The combination of knowledge found in old books and paper maps and modern information technology tools, plus a willingness to overcome multi-disciplinary and inter-organisational barriers using novel modelling methods resulted in structural model and a hydrogeological model of the Baltic Artesian Basin. An insight into the model and its construction has been provided within this book.

Hydrogeology is often classified as an applied science. Here we try to diverge from this somewhat restricted approach, considering groundwater as an interesting object of research *per se*. We took a holistic or academic look at groundwater – a slow turn-over branch of the global hydrological cycle that forms a huge in-homogeneous reservoir of water. It is inseparably confined by a matrix of even more in-homogeneous porous materials – rocks and sediments – the geological structure.

This volume is intended for three groups of readers. The first group are geology students who might found this to be a valuable stepping stone for entering the realm of geological research on the region. Various paths for further reading are given in the references. The second expected group are the practitioners – hydrogeologists - working in the region. For them this book may serve as an insight into recent academic de-

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velopments. The third group are fellow researchers not directly working in the field of hydrogeology: they may find either background information about the geology of the region or pathways for further information in the book.

The subjective nature of this book needs to be stressed: it has a strong bias towards Latvia. The relevance of the book may decrease as the distance from the country increases. Estonia as a close neighbour is covered fairy well, but Lithuania as well as other territories is considered in less detail and the reconstructions are less reliable. This means that there is still room for improvement and future research!

This collection of articles does not pretend to be comprehensive reference material on the Baltic Artesian Basin. The articles represent the scientific interests of their authors and illustrate the specifics of multidisciplinary studies.

Enjoy your reading!

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Geological evolution of the Baltic Artesian Basin

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Keywords: Baltic Basin; groundwater flow; Scandinavian Ice sheet; glacial meltwater intrusion

1. Introduction

The Baltic Artesian Basin (BAB) is one of the largest groundwater basins in Europe. It is spread over the Palaeozoic Baltic sedimentary basin and the whole territory of Estonia, Latvia, Lithuania and the Kaliningrad region of Russia, part of the Leningrad and Pskov regions of Russia, Belarus and the north-eastern part of Poland, as well as wide areas of the Baltic Sea, including Gotland Island. Its total area is 462,000 square kilometres: about 255,000 – 260,000 square kilometres being the land area with the remaining part being under the waters of the Baltic Sea.

The BAB covers a vast region that spreads across the north-western part of the core of Eastern Europe and the East European Craton (EEC). The area of the EEC formed when several small continents and island arcs collided and joined together about two billion years ago during the Paleoproterozoic. Precambrian metamorphic and igneous rocks now form the stable basement of the BAB. The entire region has a low relief, reflecting more than 600 million years of relative tectonic stability. During the long and complicated geological history, several regional tectonic elements formed within the area of the BAB such as the **Baltic Syneclise**, the **Latvian Saddle**, the **southern slope of the Baltic (=Fennoscandian) Shield**, and the **Mazurian-Belarussian Anteclise,** which is characteristic of the Cambrian – Carboniferous time. The **Middle Baltic Depression** and the **Polish-Lithuanian Depression**, formed later as well within the southern part of the Baltic Syneclise (Brangulis and Kaņevs, 2002). Throughout the Phanerozoic, the mostly low-lying territory of the Baltic States remained relatively weakly affected by the mountain-building tectonic collisions suffered by the western, northern and eastern margins of the EEC. An exception is the Caledonian Orogeny during the late Silurian – Early Devonian. After this the territory of the BAB continuously received deposits from the eroding Caledonian Mountains throughout the Devonian and Early Carboniferous. Sediments eroding from the Caledonian Mountains to the northwest washed into the sea and were deposited as layered wedges of fine debris. As sand, carbonate mud, and clays accumulated, the Devonian Baltic Basin was filled and retreated south-westward.

During most of the Mesozoic Era, the territory occupied by the BAB was mainly slightly above sea level, with the exception of the Polish-Lithuanian Depression (Paškevičius, 1997), and the Jurassic when the rising seas flooded the low-lying areas of the continent. Younger, Cretaceous and Neogene deposits are distributed in a relatively smaller part of the BAB. The whole territory of the BAB was significantly affected by several glaciations during the Quaternary.

2. Formation and structure of the territory

The structure and history of the Precambrian basement of the East European Craton in the Baltic area has recently been considerably reinterpreted (e.g., Skridlaite and Motuza, 2001; Wiszniewska and Krzemińska, 2005; Bogdanova et al., 2008; Kirs et al., 2009). Folded, deeply metamorphosed and migmatized volcanic and sedimentary rocks formed during the Palaeoproterozoic Orosirian period reflect the formation of the Svecofennian Domain from the mosaic of orogenic belts and microcontinents, starting with the island arcs (before 1910-1880 Ma, even 2145 Ma in western Lithuania) and their step-by-step amalgamation with the older Karelian Protocraton in the east. Accretion processes finished about 1800 Ma ago after Fennoscandia collided with Sarmatia in the southeast, Volgo-Uralia in the east and northeast, Amazonia in the west and unknown terrain in the southwest; after the collisions Fennoscandia became stabilized within the hypothetical supercontinent Columbia (Bogdanova et al., 2008).

Postorogenic magmatism and the formation of rapakivi plutons around the Baltic Sea (including the Riga Pluton) are connected with the rifting during the Staterian and Calymmian (Mesoproterozoic) before 1670-1500 Ma (Puura et al., 1997; Kirs et al., 2009; Motuza, 2004) suggesting the rather hilly territory of the western part of EEC at these times. Intracratonic granitoid magmatism and metamorphism occurred in eastern Poland (ca. 1500-1420 Ma ago: Bogdanova et al., 2008) and western Lithuania (1460 Ma ago: Motuza, 2004) during the Danopolonian Orogeny in the Calymmian.

There is no sedimentation evidence in the stabilized Fennoscandia during the Paleoproterozoic. The inferred oldest craton cover of the Mesoproterozoic Calymmian age is represented by the surviving fragments of the Jotnian clastic sedimentary basins in the Bothnian Gulf and the Ladoga Lake area (Puura and Klein, 1997), possibly represented by the Veiviržėnai and Baubliai Strata in Lithuania, and the Pāvilosta Strata in Latvia.

The surface of the Precambrian basement deepens in the south – south-western direction (fig.1). It is situated about 100-200 metres below sea level in northern Estonia in the vicinity of Tallinn, around 200-400 metres b.s.l. in the Valmiera-Lokno uplifted zone close to the Estonia-Latvia border and in the south-eastern part of Lithuania, on the slope of the Belarus-Mazury uplifted zone. The Precambrian basement lies about 1,000 metres b.s.l. in the northern part of the Latvian Saddle and gradually sinks to the southwest, where it reaches 2,500-3,000 metres b.s.l. in the central part of the Baltic Syneclise, and in the Baltic Sea opposite the coast of Lithuania, 4,000 metres b.s.l. in the vicinity of Gdańsk, and even 6,000 metres b.s.l. close to the Tornquist-Teisseire zone in the vicinity of Bydgoszcz. The depth of the Precambrian basement of the EEC close to Gotland and the Åland islands diminishes to 400-500 metres b.s.l. (Blazhchishin et al., 1976).

The palaeogeography of the EEC from 1,400 to 1,200 Ma ago was defined generally by rifting. Palaeomagnetic data suggest that the territory of the EEC was connected with the Amazonia block up until about 1,200 Ma (Meert and Torsvik, 2003). According to the traditional view, the EEC later became part of a supercontinent, Rodinia which supposedly formed at the end of the Mesoproterozoic approximately before 1,100 Ma and broke apart at the end of the Neoproterozoic around 800-700 Ma (Meert and Powell, 2001). During the formation of Rodinia, the EEC collided once again with Amazonia and Laurentia; the western margin of the EEC was affected by the Sve-

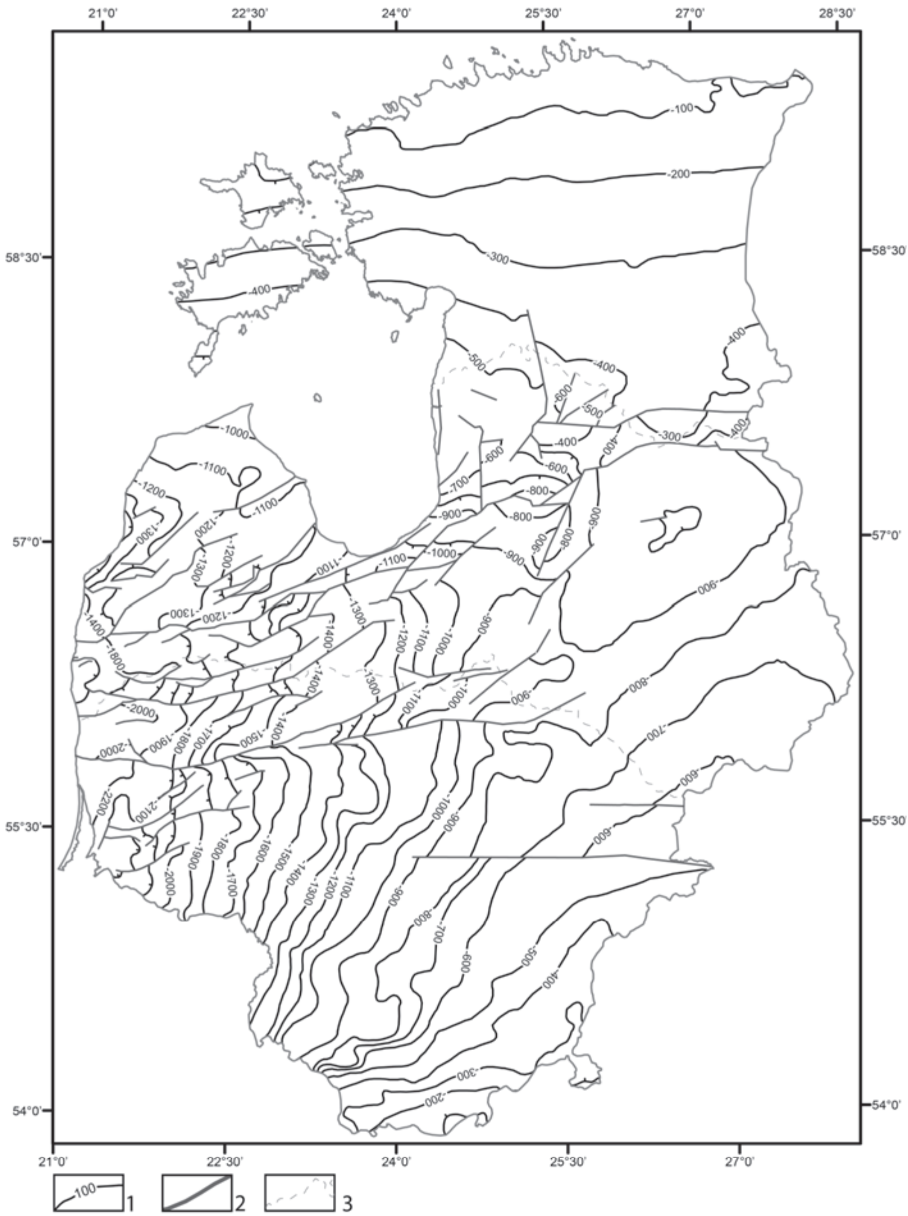

Figure 1. Top of the Precambrian basement in the Baltic States. 1, depth to basement, metres; 2, major faults; 3, state boundaries.

conorvegian Orogeny (1140 – 900 Ma). Rodinian sedimentary cover is rather poorly represented in the western part of the EEC which was affected by active tectonic processes. However widespread cover was deposited between 1,100 and 700 Ma in the central and eastern part of the EEC (Bogdanova et al., 2008). During a long-lasting period of continental environment, peneplenisation took place in the western part of the EEC and the topmost part of the basement in the territory of the BAB was significantly changed due to weathering: the thickness of the weathered crust in Latvia reaches almost 20 metres (Brangulis et al., 1998).

The large block consisting of Laurentia plus EEC formed during the initial stage of the break-up of Rodinia. Judging from palaeomagnetic data, these two continental blocks drifted together toward the South Pole during the Late Proterozoic; similarly to Laurentia, the territory of the EEC was glaciated during the Cryogenian, evidenced by the distribution of Varanger tillites in Lapland. Laurentia and Baltica began to separate at around 600 Ma with the opening of the Iapetus Ocean. After that, the separate Baltica continent (and tectonic plate) formed, which existed until the collision with Laurentia in the Caledonian Orogeny during the late Silurian – Early Devonian. The start of rifting on the Baltic margin of the EEC was marked by the 650 Ma Egersund tholeiitic dykes (SW Norway) (Torsvik et al., 1996). The Sarek dyke swarm in northern Sweden with indicators of a tholeiitic magma source dated by U–Pb zircon, dates to 608 Ma, reflecting the onset of sea-floor spreading in the Iapetus Ocean (Meert and Powell, 2001). Gudenieki alcali basalt lava (595 ± 25 Ma) in Latvia overlies rapakivi granites and anorthozites of the Riga Pluton (Birķis, 1979) and corresponds well to the Sarek dykes.

The sedimentary environment of the shallow epicontinental sea has dominated the low-lying western part of the Baltica since breaking from Laurentia and the formation of the Iapetus Ocean. The formation of thick sequences of non-metamorphosed sedimentary and volcanogenic rocks during the Neoproterozoic – Phanerozoic was affected by various orogenies. Hence, at least four structural units, separated from each other by angular unconformity, the Neoproterozoic-Lontova, Ordovician-Silurian, Devonian-Carboniferous and Permian-Cenozoic successions, are usually described, coinciding with what are referred to as the basin's Timanian ("Baikalian"), Caledonian, Variscan and Alpine stages of tectonic development, respectively.

The Timanian Orogeny during the terminal Proterozoic – Early Cambrian was the tectonic event which affected the eastern part of Baltica the most, where various microcontinental blocks in the Timan-Pechora, northern Urals and Novaya Zemlya accreted with Baltica (Cocks and Torsvik, 2005). It also probably influenced the western part of the EEC, where the boundary between the Timanian and Caledonian structural complexes in the Baltic States approximately coincided with the time of final accretion. A substantial late Cambrian orogenic event in the northwest of Baltica, called the Finnmarkian Orogeny, reached its peak during the Drumian-Guzhangian time (from 505 to 500 Ma ago; Cocks and Torsvik, 2005). It is not clear whether this orogeny affected the formation of the sedimentary succession in the territory of the BAB or not.

The Iapetus Ocean reached its widest at about the Cambrian-Ordovician boundary (Cocks and Torsvik, 2005) and from that time has been narrowing continuously. The Tornquist Ocean between Avalonia, which derived from the northern vicinity of Gondwana, and Baltica was closing and at the end of the Ordovician two of these terranes obliquely joined together into one continental block. The closure of the Iapetus Ocean resulted from the main collision between Laurentia and Baltica-Avalonia during the mid-late Silurian, and as a result the Scandian Caledonides formed in the eastern part of the collision front and the supercontinent of Laurussia (or Euramerica) appeared. The Caledonian Orogeny substantially affected the territory of the BAB due to variously directed movements of tectonic blocks, significant erosion of the Silurian and partly Ordovician deposits, and provided space for the sedimentary basins which developed during the Devonian and Carboniferous in the Baltic area.

Some time after the formation of Laurussia, the southern part of Europe was involved in the late Palaeozoic Variscan Orogeny, which cut off the southern margin of the former Baltica. The Variscan Orogeny resulted in the amalgamation of Laurussia and the huge Gondwana Terrane, as well as the complex set of peri-Gondwanan terranes, into the Pangea supercontinent by the end of the Permian (Torsvik and Cocks, 2004). Approximately at the same time the eastern margin of the former Baltica was deformed during the Late Carboniferous Uralian Orogeny. In contrast to the Variscan Orogeny, which induced the termination of marine sedimentation in the area of the BAB, the Uralian Orogeny affected mostly the eastern part of the EEC.

Starting from the Jurassic, the time of the breakup of Pangea, the EEC formed the integral part of the vast Eurasian Plate, today creating a large part of its passive western margin (Bogdanova et al., 2008). Hence all sedimentary formations of the Permian-Cenozoic were deposited on the low-lying relief of the surface of mainly Devonian and Carboniferous sedimentary successions.

3. Mesoproterozoic succession

There are only small fragments of probably Mesoproterozoic formations in the territory of the BAB. The tectonically deformed **Veiviržėnai Strata** are composed of volcanomictic sandstone and gravelstone in their lower part, covered by medium-grained sandstone in the middle part and conglomerates with gneiss, quartz and basalt-like pebbles and breccias (Paškevičius, 1997). The total thickness reaches 23 m. The Veiviržienai Strata overlay Palaeoproterozoic rocks of the Western Lithuanian Granulite Domain and are capped by the Baubliai Strata. Usually the Veiviržėnai Strata have been correlated with the Hogland series of the Subjotnian (Paškevičius, 1997), but the composition of basalt-like pebbles and breccias can not exclude the interpretation of these strata as younger than the Calymmian rocks of Suursaari Island and the Undva section of Estonia (Kirs et al., 2009) or even the Ediacaran Gudenieki lava of Latvia.

The discordantly overlying 14 metres thick **Baubliai Strata** consist of quartz sandstone intercalating with siltstone without large fragments of volcanic rocks. The exact age of the Baubliai Strata are not known and are variously interpreted as Neoproterozoic (Paškevičius, 1997) or Mesoproterozoic, in the latter case correlating these deposits with the Scandinavian Jotnian sandstones (Jankauskas, 2004b).

The probably volcanoclastic **Pāvilosta Strata** composed of quartz-porphyry and sandstone of quartzite type with an admixture of tuff represent a body of similar age in Latvia. The composition of these rocks resembles that of the Subjotnian (Calymmian) and Jotnian (Ectasian) acidic volcanic rocks of Suursaari (Birķis, 1979). The Quartz-porphyry has been strongly weathered, and therefore its isotopically dated age (1050 ± 30 Ma) is considered to be substantially reduced.

4. Neoproterozoic succession

4.1. Ediacaran

Various deposits formed during the time span from the formation of the Iapetus Ocean to the Timanian Orogeny, were previously reported as the "Baikalian structural complex". However, although the term "Baikalian" has still sometimes been applied to events within Baltica (Brangulis and Kaņevs, 2002; Brangulis et al., 1998; Suveizdis, 2004), it is now clear that the use of the term should be confined only to Siberia and the term "Timanian complex" is preferable (e.g., Shogenova et al., 2009). This complex discordantly overlies the Precambrian basement and consists of the Ediacaran volcanoclastic and clastic deposits united into several stratigraphic units, as well as the so called blue clay of the lower Cambrian Lontova Formation covering the largest part of the Baltic States.

The Ediacaran Period was officially ratified in 2004 by the International Union of Geological Sciences as the last geological period of the Neoproterozoic (Knoll et al., 2004). The Ediacaran Period overlaps, but is shorter than the Vendian Period, which was proposed in 1952 and has previously been widely used for the whole territory of the EEC and Siberia (Sokolov, 2011). To avoid problems in correlating the Vendian formations with the Cryogenian, Ediacaran and Cambrian systems, the name Ediacaran is accepted here for all Neoproterozoic rocks despite the fact that the correct geochronological data are mostly missing.

Ediacaran rocks are distributed in the so called East Baltic Depression coinciding with a large part of Estonia, the eastern part of Latvia and eastern Lithuania, as well as having been reported from a small area of western Kurzeme. Rocks of the same age are widely distributed in Belarus and Russia. The most complete section of Ediacaran rocks occurs in eastern Lithuania where these are represented by the Merkys, Jašiūnai, Rūdninkai, Pagiriai, Skynimiai and Vilkiškiai formations, united into the Volyn' and Valdai regional series (Jankauskas, 2004a). A well defined sedimentary break between the Rūdninkai and Pagiriai formations separates the Volyn' and Valdai regional series in Lithuania.

The oldest, the **Merkys** Fm, is the up to 23 metres thick section of reddish brown gravelite fanglomerates with siltstone interlayers, which overlie the Precambrian basement. Age determination is based on the correlation with analogous rocks from northern Belarus (Jankauskas, 2004a). The overlying **Jašiūnai** and **Rūdninkai** formations are composed of rhythmic successions of horizontally bedded and cross-stratified reddish brown arcosic conglomerate (in Jašiūnai Fm with up to 2.5-3 centimetres large pebbles), gravelstone and sandstone; the Rūdninkai Fm also contains silty material with an admixture of kaolinite up to 40% in its upper part. The Jašiūnai Fm (up to 40-50 metres thick) is distributed over the larger area than both the Merkys and Rūdninkai (20-28 metres thick) formations.

It is rather complicated to correlate various stratigraphical units within the Volyn' Regional Series even in a relatively small area such as the Baltic States due to the lack of good age indicators. Possibly, deposits corresponding to the Volyn' Regional Series are missing in central Lithuania (Jankauskas, 2004a) and Estonia (Pirrus, 1996). In Latvia, only the Gudenieki Strata in the western region correspond to the Volyn' Regional Series; the lack of palaeontological or other evidence does not allow one to make the correlation between the Krāslava and Zūras strata with the Volyn' or Valdai regional series with confidence (Brangulis et al., 1998).

The **Krāslava** Strata are distributed in south-eastern Latvia between the underlying Precambrian basement and the overlying Kotlin Formation, which corresponds to the Valdai Regional Series. The Krāslava Strata closely resembles the Merkys-Rūdninkai succession in composition and consists of weakly cemented, poorly sorted reddish or yellowish brown gravelstone and sandstone with rare interlayers of silt and silty clay, as well as an admixture of volcanoclastic material. The thickness of the Krāslava Strata increases from several metres in the north to 96 metres in the very south-east of Latvia.

Ediacaran rocks distributed in a small isolated area of western Latvia and the neighbouring Baltic Sea are represented by the Gudenieki and Zūras strata. **Gudenieki** alcali basalt lava (595 ± 25 Ma), resembling limburgite in its chemical composition, overlies the rapakivi granites and anorthozites of the Riga Pluton (Brangulis et al., 1998). The age of the **Zūras** Strata is not well defined. These strata reach 30 metres in thickness and are subdivided into the lower volcanoclastic bed and the upper, clastic bed. The volcanoclastic bed contains volcanomictic sandstone, gravelstone and conglomerate with interlayers of sandstone, gravelstone and clay in the upper part. The clastic bed consists of siltstone and fine sandstone with interlayers of gravelstone, conglomerate and clay. The clastic bed yields *Laminarites*-type algal laminae and acritarchs *Leiosphaeridia* sp., evidencing the Valdai age of this part of the section (Brangulis et al., 1998).

Deposits corresponding to the Valdai Regional Series are more widely distributed in the area of the BAB including the Pagiriai, Skynimiai and Vilkiškiai formations in Lithuania and the Gdov, Kotlin and Voronka formations in Latvia and Estonia (Jankauskas, 2004a; Brangulis et al., 1998; Mens and Pirrus, 1997); as stated above, the upper part of the Zūras Strata most probably corresponds to the Valdai Regional Series. In the Baltic area, the Valdai Regional Series corresponds to the Kotlin Regional Stage (RS), which is represented by siliciclastic rocks accumulated in cool and humid conditions (Pirrus, 1992). The Kotlin RS represents the high-order cycle of sedimentation (Mens and Pirrus, 1997) with multicoloured sandy-silty poorly sorted material at the base (Gdov and Pagiriai formations), grey-coloured clayey deposits in the middle (Kotlin and Skynimiai formations), and variegated silty-sandy material in the upper part (Voronka and Vilkiškiai formations).

In Estonia and Latvia, the **Gdov** Formation lies on the Precambrian basement, with the exception of south-eastern Latvia. Its thickness varies from 0.2 to 58 m. The formation mainly consists of poorly sorted and weakly cemented sandstone with lenses of gravelstone, siltstone and clay.

The **Koltin** formation is dominated by thinly laminated grey and greenish clay ("Laminarites" Clay) with intercalating siltstone or very fine-grained sandstone. It is present in Latvia and eastern Estonia up to the Otepää – Viljandi – Rakvere line, with its thickness reaching 45-54 m.

The **Voronka** Formation is distributed in eastern and northern Estonia and in eastern Latvia. It occurs between the kaolinite weathering crust of the underlying Kotlin Fm and the overlying Cambrian Lontova Fm. The Voronka Fm consists of various siliciclastic deposits coarsening upwards: clayey siltstone, siltstone, well-sorted sandstone with clay and gravelstone interlayers. The clay fraction is dominated by kaolinite. The thickness of the formation reaches 40 m.

5. Palaeozoic succession

5.1. Cambrian

In general, the Cambrian deposits in the BAB represent the continuation of the transgression onto the peneplained Precambrian basement, which already began during the Ediacaran. The lack of coarse clastic deposits, and the thinness and extensive lateral range of facies suggest that the terrane was relatively low in topography. The oldest Cambrian (Terreneuvian) deposits in the area of the BAB correspond to the Rovno RS (fig. 2) and are distributed only in Lithuania (Jankauskas and Laškova, 2004). The **Rudamina** Fm consists of dark grey and greenish grey clay intercalated by sandstone, gravelstone and siltstone with acritarchs and annelid fossils. It discordantly overlies the Precambrian basement and Ediacaran rocks of various ages, and is about 44 metres thick (Paškevičius, 1997). Analogical deposits in eastern Latvia previously have been attributed to the lowermost part of the Lontova Fm.

The overlying deposits of the Lontova and Voosi formations are distributed almost over the whole territory of the Baltic States. The **Lontova** Fm "Blue Clay" consists of laminated greenish grey clay and silty clay with interbeds of coarse- to fine-grained sandstone at the base and siltstone at the top. A thick weathering crust (3-5 m) covers this clay. The Lontova clay forms a confining bed of regional importance. It reaches its largest thickness of 125 metres in south-eastern Latvia; westwards it is laterally replaced by the Voosi Fm (Mens and Pirrus, 1997). The **Voosi** Fm consists mostly of quartzose sandstone in the Estonian islands while clay, siltstone and fine-grained sandstone make up the upper part of the formation in the mainland of Estonia. Its thickness ranges from 14.6 to 72 m.

The overlying Caledonian structural complex corresponds to the post-Lontova Cambrian, Ordovician and Silurian deposits. Traditionally the Early Devonian Gargždai Group is also included in the Caledonian complex, despite the fact that it concordantly overlies the Silurian (Přidolian) deposits only in the axial part of the Baltic Syneclize, in south-western Lithuania and western Latvia (borehole Oviši-94). However, the Gargždai Group lies upon the Wenlock in the Latvian Saddle and southern slope of the Fennoscandian Shield and even the Ordovician in the vicinity of Peipus Lake in Estonia. Such an important stratigraphic break suggests the need for additional analysis on the inclusion of the Gargždai Group into the Caledonian complex. The Caledonian complex reaches its largest thickness of 1,000-1,200 metres in western Lithuania; it varies from 800-1,000 metres in north-western Lithuania to less than 200 metres in northern and eastern Estonia.

The oldest deposits of the Caledonian complex belong to the lower part of the Dominopole RS which corresponds to the Oviši and Sõru formations distributed in the restricted area of north-western Latvia and Estonia (islands of the Western Archipelago). The precise correlation of the series of new, four-fold subdivisions of the Cambrian, and strata in the Baltic area is the subject of further studies, therefore the precise position of the boundary between the Terreneuvian and Series 2 is not known; most probably it lies between the Dominopole and Ljuboml' RS. During the late Dominopole time the sedimentary basin gradually widened until at the end of the Terreneuvian – beginning of the Series 2, it occupied almost the whole territory of the Baltic States.

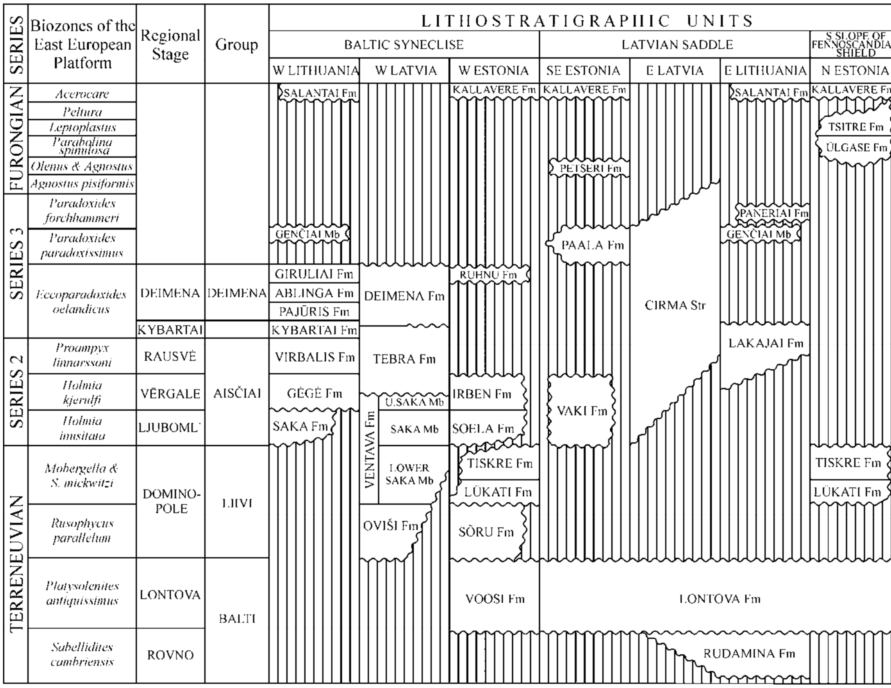

Figure 2. Stratigraphic chart of the Cambrian succession in the Baltic States (based on Mens and Pirrus, 1997 for Estonia, Gailīte et al., 2000 for Latvia, Jankauskas and Laškova, 2004 for Lithuania).

The Cambrian and Early Ordovician succession deposited on the Baltic Basin area is dominated by siliciclastics, probably indicating the moderate to high latitude position of the continent. Cambrian rocks outcrop only along the Baltic Glint, but they are mostly overlain by younger strata. The section contains many stratigraphic gaps, and therefore the precise correlation and age determination of various stratigraphic units is a matter of discussion.

The upper Terreneuvian **Oviši** and **Sõru** formations discordantly overlie the Precambrian basement. Fine-grained quartz and quartz-feldspar sandstone and siltstone, interbedded with clay, conglomerate and gravelstone, dominate the formations, which are 58-60 metres thick (Brangulis et al., 1998; Mens and Pirrus, 1997).

The **Ventava** Fm consisting of the three members is distributed in western Latvia, where it is 45-63 metres thick. Greyish green or reddish brown variegated clay with siltstone and sandstone interbeds dominate the **Lower Saka** Mb, **Lükati** and **Saka** formations. The fine-grained sandstone with rare clay forms the **Saka** Mb and **Tiskre** Fm.

Most probably the boundary between the Terreneuvian and Series 2 corresponds to the gap between the Tiskre Fm and Soela Fm in Estonia, the Saka and Gėgė formations in Lithuania, and within the Saka or below the Upper Saka Mb in Latvia. Fine-grained siliciclastic and clay deposits dominate the Series 2 in the Baltic area. Siltstone and clay deposits dominate the **Upper Saka** Mb, whereas fine-grained sandstone and siltstone with clay interbeds are widely distributed in part A of the **Gėgė** Fm, as well as in the **Soela** Fm. The **Tebra**, **Virbalis** and **Irben** formations contain greenish grey clay and siltstone with sandstone interlayers. Silty clay, siltstone and fine-grained sandstone with goethite and chamosite ooids from the B part of the Gėgė Fm, the lower part of the Tebra Fm and Irben Fm are considered to be a good regional marker. The **Vaki** Fm distributed in south-eastern Estonia is probably a shallow-water equivalent of the Soela and Irben formations, consisting of glauconite-bearing fine-grained sandstone with thin interlayers of argillaceous rocks (Mens and Pirrus, 1997).

The **Cirma** Strata, and the **Lakajai**, **Paneriai** and **Paala** formations mostly of Series 3 age after the significant break, overlie the Precambrian basement or the Terreneuvian Lontova clay with angular unconformity. The Cirma, Lakajai and Paneriai units yield rather poor fossil assemblages which do not allow for the precise correlation with units in the western part of the Baltic Basin. All these units are practically identical in rock composition, consisting of weakly cemented sandstone with interlayers of siltstone and rare argillaceous rocks; only the Paneriai Fm differs with a larger content of silty and clayey rocks.

The **Kybartai** Fm consists of argillaceous rocks and glauconitic sandstone. Fine-grained sandstone with rare interlayers of siltstone and clay of the **Deimena** Fm concordantly overlies the deposits of the Kybartai or Tebra formations. The **Ruhnu** Fm differs from the Deimena Fm with a smaller content of silty and clayey components.

Deposits of the upper part of the Cambrian in the Baltic territory are distributed in a restricted area of eastern Lithuania, northern Latvia, as well as northern and south-eastern Estonia and may well correspond to the Furongian Series because of the stratigraphic gap between the Paala Fm (Middle Cambrian of the previous chart) and the overlying Petseri, Ülgase, Tsitre formations and the lowermost part of the Kallavere formation; the age of the Salantai Fm and some parts of the Cirma Strata have been determined from typical upper Cambrian obolid brachiopods and acritarchs respectively (Jankauskas, 2004b; Brangulis et al., 1998). All lithostratigraphic units of the Furongian age consist of fine-grained quartz sandstone and siltstone with rare interlayers of clay.

The boundary between the Cambrian and Ordivician lies within the **Kallavere** Fm evidenced by distribution of conodonts. Nevertheless, the Kallavere Fm has usually been treated as the base of the Ordovician. The quartzose sandstone with interbeds of dark argillite and coquina of abundant brachiopods with phosphatic valves dominate the Kallavere Fm distributed almost all over Estonia. The **Salantai** Fm of Lithuania most probably corresponds with the lowermost Kallavere Fm.

The Cambrian sequence and Lower Ordovician sandstones of the Kallavere Fm are united into the Cambrian aquifer complex, which is distributed almost all over the territory of the Baltic Basin. The depth of the upper surface of the Ordovician-Cambrian aquifer complex ranges from 10-20 metres in northern Estonia to 1,800-2,000 metres in south-western Lithuania, the central part of the Baltic Syneclise.

5.2. Ordovician

Deposits of all three series of Ordovician are widely distributed in the whole area of the Baltic Basin (fig. 3), extending to Belarus and Poland in the south and the vicinity of Moscow in the east. Ordovician rocks usually discordantly overlie Cambrian siliciclastic deposits, and are overlain by the Silurian in a wide area, except northern and eastern Estonia, and the south-eastern areas of Latvia and Lithuania.

During the Early and Middle Ordovician, the territory of the BAB was slowly subsiding and covered by a shallow sea with slow sedimentation of mainly siliciclastics (in the Early Ordovician) and carbonates (in the Middle Ordovician). Due to Baltica drift from high to low latitudes, carbonate rocks dominate the sequence starting from the Middle Ordovician.

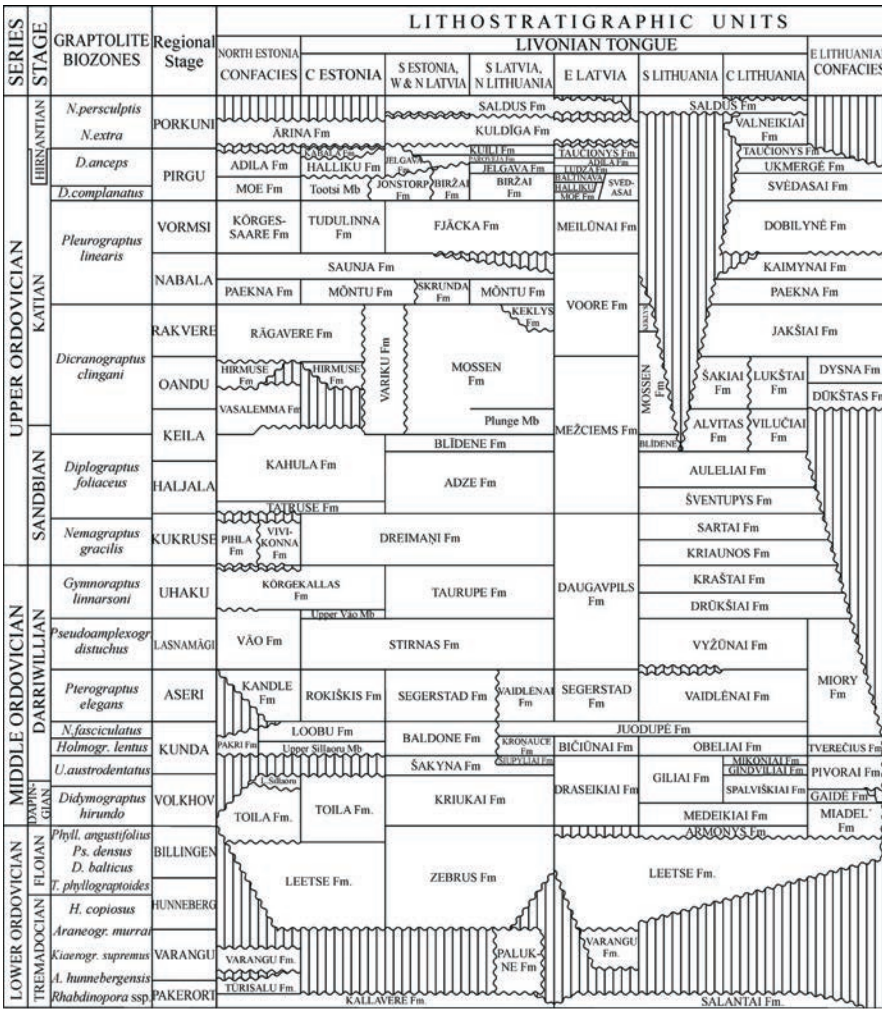

Figure 3. Stratigraphic chart of the Ordovician succession in the territory of the Baltic States (based on Meidla et al., 2008 for Estonia, Gailīte et al., 2000 for Latvia, Paškevičiene and Laškovas, 2004 for Lithuania).

Two main elements of the Baltic Ordovician Basin have been recognized and introduced in the middle of the 20th century: the central and marginal. The central or Swedish-Latvian structural-facies zone (Männil, 1966), or confacies belt (Jaanusson 1976), sometimes called the Livonian zone (Paškevičius, 1994) or Livonian Tongue, coincides with part of the Scandinavian Basin (Harris et al. 2004) and is characterized by relatively deep-water deposits of silt, limestone, dolomite and clay. The marginal or Estonian-Lithuanian Confacies Belt make up the Estonian and Lithuanian shelf and coincides with the distribution of mainly shallow-water carbonates.

The Lower Ordovician is dominated by sandy (Kallavere, Salantai, Leetse formations) and argillaceous (Türisalu, Paluknė, Varangu formations) deposits or the intercalation of sandy and clayey rocks (Zebrus). The transition from siliciclastic to carbonate rocks is marked by the appearance of calcareous beds in the upper part of the Leetse and Zebrus formations, and the Armonys Fm which consists of limestone and dolomite. The Middle Ordovician is mainly composed of limestone succession which has been formed as cold-water carbonates deposited in a sediment starving shallow marine basin (Meidla et al., 2008). The Upper Ordovician succession demonstrates the increasing rates of sedimentation due to increased carbonate production. The section is chiefly composed of limestone with intercalations of the kukersite oil shale mainly in the Kukruse Regional Stage in the Estonian Confacies Belt.

The thickness of the Ordovician deposits reaches 180 metres in southern Estonia, 240-250 metres in western and central Latvia (Jelgava depression), and 230-240 metres in eastern Latvia and Lithuania. The upper surface of the Ordovician rocks is roughly parallel to the Precambrian basement. It deepens from sea level in northern Estonia, to 200-400 metres below sea level in eastern Latvia and Lithuania and reaches 1,800-2,000 metres below sea level in western Lithuania.

5.3. Silurian

Silurian deposits are widely distributed in the Baltic Basin, except south-eastern Latvia and Lithuania and the largest part of Estonia. During the Silurian Period, the Baltica continent, later the East European Platform as an integral part of the Euramerica continent, was located close to the equator, slowly moving northward. The pericratonic Baltic Basin was characterised in its marginal parts, in Estonia, south-eastern Latvia, as well as south-eastern and central Lithuania, by various tropical shelf environments and diverse biotas. Due to the closure of the Iapetus Ocean and the oblique collision of Baltica and Eastern Avalonia, a flexural foreland basin depression was formed in the axial part of the Baltic Basin (Poprawa et al., 1999), where mainly clayey deposits were accumulated during the Silurian.

Silurian rocks are distributed under the unevenly thick Quaternary cover in a wide belt from Saaremaa Island in the west to Lake Peipsi in the east. In south-eastern Lithuania, the Silurian deposits are also covered by 80-90 metres thick Quaternary deposits, or in places by Permian. Devonian siliciclastic rocks lie over the Silurian deposits elsewhere. Due to the gradual infilling of the basin from north-east to south-west, the oldest Silurian rocks are distributed in the northern and eastern part of Estonia, as well as south-eastern Latvia and Lithuania, whereas younger strata cover smaller areas. The most complete sections have been found in the western part of Latvia and Lithuania, where Přidolian rocks are concordantly overlain by the Lower Devonian deposits (Narbutas et al., 1981). The thickness of the Silurian succession here reaches 830-850 metres and the upper surface lies about 1,200-1,250 metres below sea level.

The Silurian succession consists of shallow-water limestone and dolomite with diverse shelly fauna in the northern and south-eastern areas, and more deeper-water facies represented mainly by argillaceous deposits, from calcareous clay and marlstone to graptolithic shales in the central part of the basin (fig. 4).

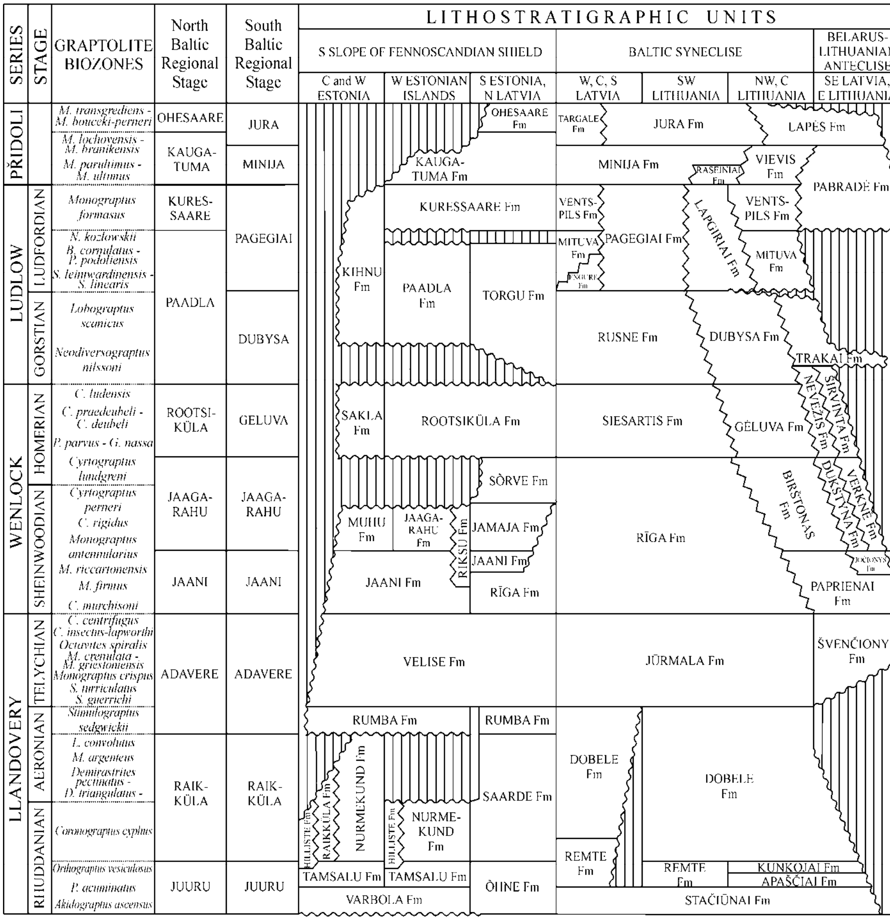

Figure 4. Stratigraphic chart of the Silurian succession in the territory of the Baltic States (based on Hints, 2008 for Estonia, Gailīte et al., 2000 for Latvia and Lapinskas, 2004 for Lithuania).

5.4. Water in the Ediacaran-Silurian rocks

The United Cambrian-Ediacaran aquifer in south-eastern Lithuania corresponds to all deposits of the Timanian complex including the lower part of the Lontova Fm. In the eastern part of the Latvian-Lithuanian boundary area and eastern Estonia there are two aquifers: Gdov and Voronka. The Gdov aquifer in Estonia corresponds to the Gdov Fm (Perens and Vallner, 1997), whereas in Latvia it includes the Gdov Fm and the Krāslava Strata; the Kotlin aquitard isolates the Gdov aquifer from the Voronka aquifer. The Voronka aquifer is distributed in northern Estonia and eastern Estonia and Latvia; it coincides with the Voronka Fm and the lower part of the Lontova Fm. The Cambrian-Ediacaran aquifer in the whole area of the East Baltic is isolated from younger aquifers by the Lontova regional aquitard.

The Ordovician and Silurian deposits form the ***Silurian-Ordovician aquitard*** of regional importance (Perens and Vallner, 1997). Despite the fact that carbonate rocks dominate the Silurian and Ordovician formations, the ***Silurian-Ordovician aquifer*** system is an important source of water in Estonia only in the area north of the Pärnu-Polva line and on the islands of the West-Estonian Archipelago, as well as in south-east Lithuania, in the Vilnius area. It consists of various limestones and dolomites with argillaceous interlayers. The upper, approximately 30-35 metres thick portion of the rocks forming the aquifer system, is rather cavernous, with many cracks and fissures; deeper lying carbonate rocks contain less fissures and cracks, gradually turning into an aquitard. The best and wide Ordovician aquifers intercalating with the aquitards are as follows (from top to base): the Nabala-Rakvere aquifer, the Oandu aquitard, the Keila-Jõhvi aquifer, the Jõhvi-Idavere aquitard, the Idavere-Kukruse aquifer and the Uhaku aquitard (Perens and Vallner, 1997). The deposits of the Adila Fm (Pirgu RS), rocks corresponding to the Silurian Raikküla RS and some other formations also could be used as aquifers. The well defined aquitard in the northern part of Estonia is formed by the Lower Ordovician Türisalu, Varangu and Leetse formations, as well as Toila Fm. Farther to the south, the aquitard includes all Silurian and Ordovician rocks, reaching its maximum thickness of about 250-350 metres close to the southern border of Estonia.

The Silurian-Ordovician aquifer has also been found in the south-eastern part of Lithuania on the slope of the Mazurian-Belarussian anteclise, where it is formed of porous and cavernous carbonate rocks. The thickness of the aquifer reaches 150-200 metres, and its upper surface lies 80-250 metres below the ground surface. The upper portion of the Ordovician-Silurian deposits contains more water, but the water content in the deeper layers is uneven.

The water content in the other areas of the Baltic Artesian Basin is sporadic and corresponds to the cracked and fissured deposits in the fault zones and lenses of biodetrital, biomorphic and biohermal limestones.

5.5. Devonian

The Devonian sequence is distributed across almost all the Baltic Basin area (Poprawa et al., 1999) and reaches a maximal thickness of 1,000 m in the north-western part of Lithuania. It thins out towards the north and the south-east. Devonian deposits are absent in most of Estonia and southern Lithuania.

All of the Devonian series and stages are present in the area of the south-east Baltics, however, its stratigraphical completeness varies from place to place (Fig 5).

The Devonian thickness map (Paškevičius, 1997) shows that in Estonia the thickness of the Devonian deposits gradually increases southwards and reaches 400 m in its south-eastern corner. Devonian deposits are absent in its central and northern part, however, in the north-eastern part they stretch almost to Narva. Devonian deposits cover the whole land area in Latvia, with the thickness reaching approximately 800 m in the south-western part, decreasing northwards to 200 m and to approximately 250 m in the south-east. The Devonian deposits are at their maximum thickness in western Lithuania, close to Gargždai, where they reach 1,000 m. This area and south-western Latvia correspond to the central part of the main Devonian depocenter within the Baltic

Basin - the Latvian-Lithuanian depression. The thickness of the Devonian deposits in Lithuania decrease in its northern part to 800 m, in the eastern part to 100 m, and decrease sharply in a southerly direction. Devonian deposits are absent in the southern part of Lithuania (Paškevičius, 1997).

5.5.1. Lower Devonian

The Lower Devonian deposits differ in that they consist of siliciclastics, but in the eastern part - dolomitic marls are present. The lower erosional boundary of the Devonian in most of the south-east area of Baltic countries is sharp, and a transitional boundary between the Silurian and the Devonian without considerable gaps exists only in western Lithuania, south-western and north-western Latvia, where the most complete geological sections are present (Paškevičius, 1997).

The lower part of the Lower Devonian, the Lochkovian Stage, in the south-east Baltics occurs in three areas. The largest is the central and southern part of the Baltic Syneclise (western and central Lithuania), where the oldest Devonian deposits reach a considerable thickness (more than 220 m), and the section is the most complete there. The Lochkovian Stage here is divided into 2 regional stages – the **Tilžė and Stoniškiai**, each of them represented by one formation with the same name. The Tilžė regional stage (RS) (and Fm) is composed of siltstone, sandstone, clay, marl, clayey and sandy dolomite. The clayey to silty deposits are often reddish-brown. The Stoniškiai RS (Fm) has a similar composition, but the amount of sandy material is larger than in the Tilžė RS. Pebbles of carbonate rocks are present in the sandstones (Paškevičius, 1997). The deposits of the Tilžė RS are homogeneous or have a planar lamination, and the distribution of carbonate admixture here is uniform. The deposits of the Stoniškiai RS have irregular relationships of clastic and carbonate material and therefore, nodular and cellular structures are present (Kurshs, 1992). Outside the central part of the Baltic Syneclise, it is difficult to distinguish the two chrono- and lithostratigraphical units, therefore one lithostratigraphical unit – the Gargždai Group, has been defined (Kurshs, 1992).

From the north-eastern corner of Lithuania, the Lochkovian deposits stretch out from the Baltic Syneclise to the Latvian Saddle (eastern Latvia), where they form a striking north-south belt of 50-70 km width. The thickness there reaches 60 m (in Madona-93 borehole; Narbutas and Ljarskaja, 1981). In eastern Latvia, these deposits are richer in dolomitic marl (Kurshs, 1975). In south-eastern Estonia, only the Tilžė RS is present in the Lochkovian, and it is represented by grey and purplish-grey siltstones and sandstones with interlayers of clay and dolomite (Kleesment and Mark-Kurik, 1997a). V. Kuršs has noted that the lower part of the Gargždai Group is present in eastern Latvia as well (Kurshs, 1975). The thickness of the Tilžė RS changes from 2 to 21.7 m (in Laanametsa borehole; Narbutas, 1981).

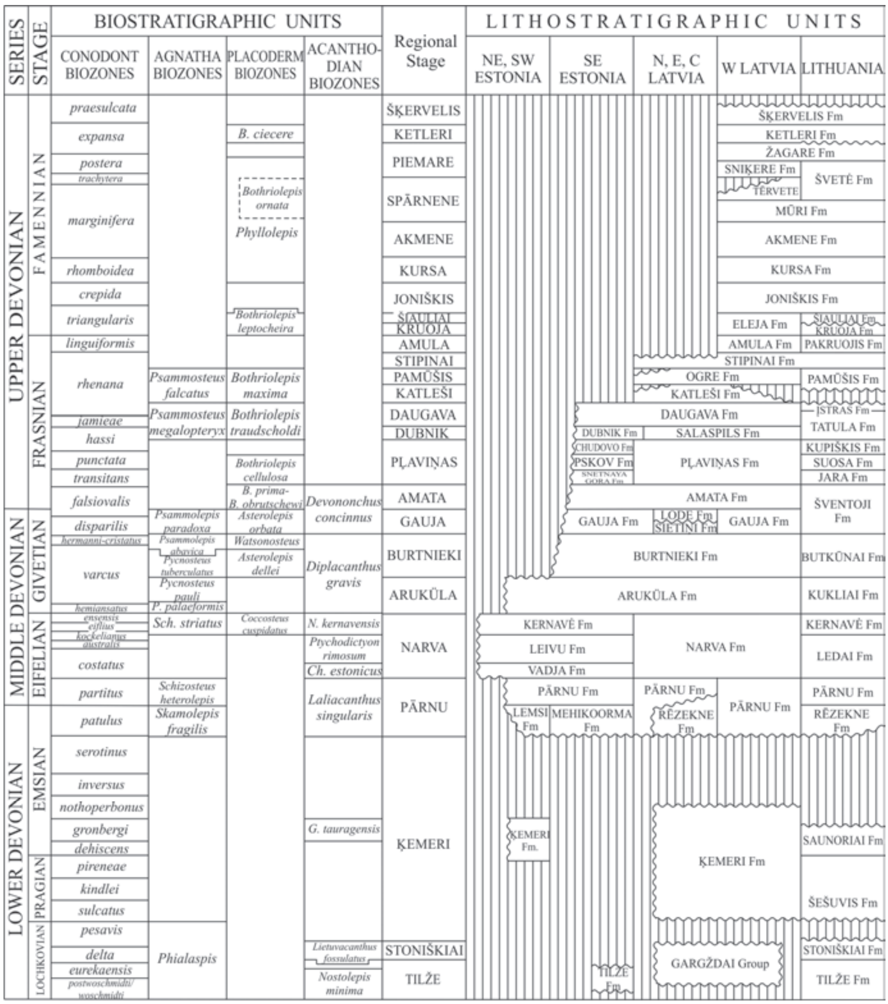

Figure 5. Stratigraphic chart of the Devonian succession of the south-east Baltic States (based on Kurik & Põldvere 2012 for Estonia, Stinkulis, 2004 with contribution of Lukševičs for Latvia, Narbutas, 2004 for Lithuania).

During the Lochkovian time, the filling of the basin, which had already developed in the Silurian, continued. The deepest part of this basin was located in the Baltic Syneclise, which is suggested by the greatest thickness, the most complete geological section and by the composition of deposits, dominated by carbonate, clay and silt material (Kleesment, 1997; Kurshs, 1992). According to V. Kuršs (Kurshs, 1992), during the Gargždai time, the basin was a large restricted lagoon. Due to the lack of outcrops, the data on palaeocurrent directions is absent, except for an attempt to measure the cross-strata dip azimuths in drill cores oriented by the palaeomagnetic method (Gerashenko et al., 1981).

The Tilžė and Stoniškiai RS in the stratigraphic chart are followed by the **Ķemeri**

RS, which belongs to the Lower Devonian – Pragian and Emsian Stages, except in its uppermost part (Paškevičius, 1997). The distribution of the Ķemeri RS is considerably more regular than that of the Tilžė and Stoniškiai RS and stretches from western and central Lithuania through the largest part of Latvia (except the eastern part) to the very southernmost part of Estonia (Kurshs, 1975). In Latvia and south-western Estonia, the Ķemeri Fm, but in Lithuania the Viešvilė Group, correspond to the Ķemeri RS (Paškevičius, 1997; Narbutas, 2004). The basal part of the Ķemeri Fm is marked everywhere by conglomerates or sandstones with pyrite and dolomite cement (Ljarskaja, 1981). In western Latvia the lower part of the Ķemeri Fm is composed of alternating sandstone, siltstone and clay. Dark-grey micaceous sandstones and siltstones with abundant plant remains are present there among the sandy beds. The upper part of the section is dominated by greyish-violet clayey siltstones with inclusions of dolomite (Ljarskaja, 1981). In central and north-eastern Latvia, the Ķemeri Fm is dominated by sandstones (up to 70%). Sandstones and siltstones with plant remains are present in the lower part of the formation here as well. Siltstones with a carbonate admixture gradually changes eastwards to planar-laminated non-carbonate varieties. The content of sandy fraction in the deposits of the Ķemeri Fm increases to the north-east until it reaches more than 90% in north-eastern Latvia and neighbouring south-western Estonia (Kurshs, 1992).

During the Ķemeri time, clayey and silty deposits (slightly dominant) and sandy material accumulated in the relatively deeper part of the basin, in western Latvia and Lithuania. In central and eastern Latvia and central and north-eastern Lithuania the basin was shallower and sandy sediments dominate the section (Kurshs, 1975).

The boundary between the Gargždai Group and the Ķemeri Fm is suggested to correspond to a boundary between the Caledonian (Fig. 6) and the Hercynian (Variscan) structural complexes (tectonic cycles) as the deposits of the Gargždai age and below are eroded by the end of the Gargždai time and the Lower Palaeozoic to Gargždai sedimentary cover has more complex tectonic structure than the younger Devonian sequence (Brangulis and Kaņevs, 2002).

5.5.2. Lower to Middle Devonian

The deposits of the Gargždai Group and Ķemeri RS are covered by more widespread upper Emsian (Lower Devonian) to lower Eifelian (Middle Devonian) deposits. It is divided into two regional stages – **the Rēzekne RS** (upper part of the Emsian) and **the Pärnu RS** (lower part of the Eifelian) (Kleesment and Mark-Kurik, 1997a; Paškevičius, 1997) though stratigraphic subdivision remains problematic outside the eastern part of the south-east Baltic States and south-western Estonia and north-western Latvia (Kleesment, 1981; Kurshs, 1992; Kleesment and Mark-Kurik, 1997a; Kurshs and Stinkulis, 1998). In other areas, due to a similar lithology (mainly siliciclastics) and poor palaeontological characteristics, these regional stages are difficult to distinguish and they are often mentioned as the Rēzekne-Pärnu undivided RS.

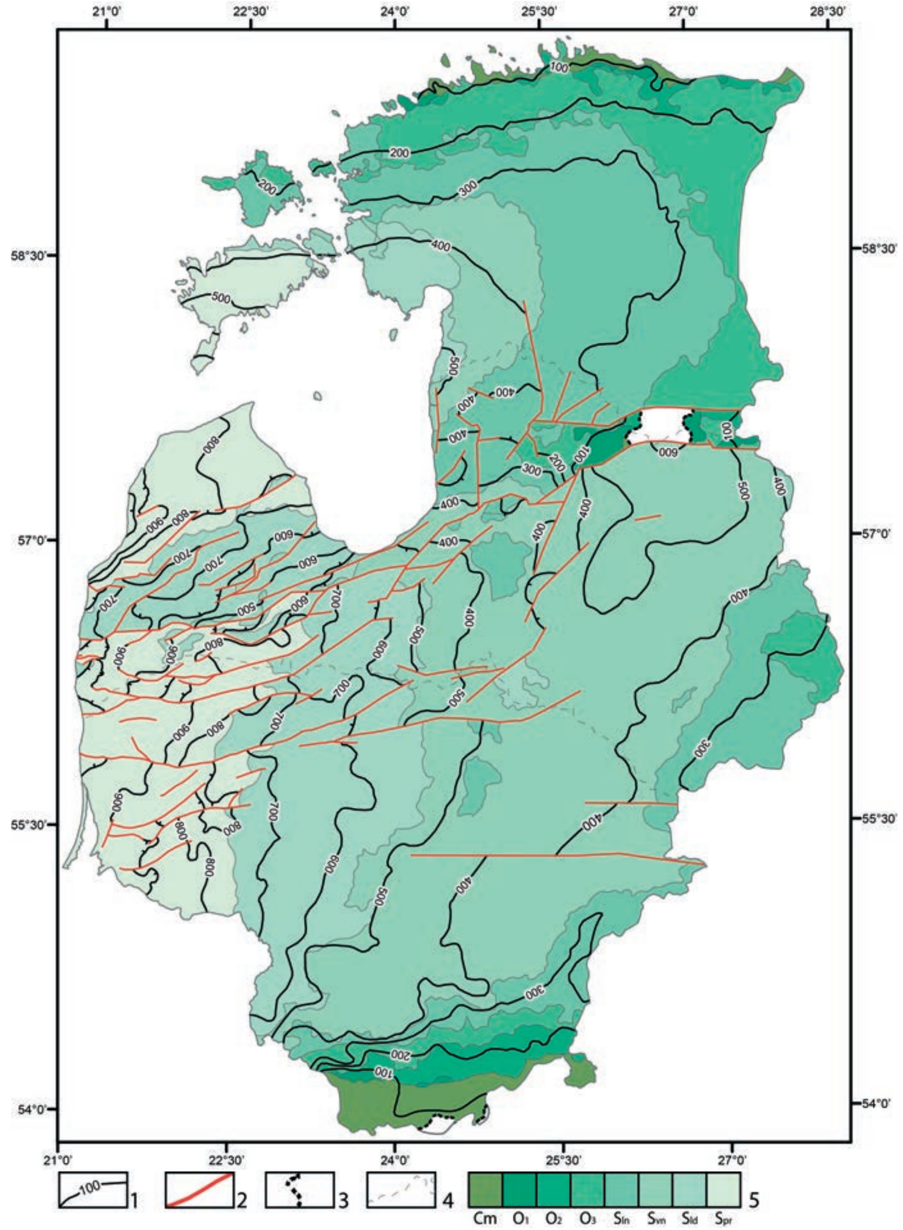

Figure 6. The geological and thickness map of the Caledonian structural complex (without the Devonian Gargždai Group): 1 – isopachs; 2 – faults; 3 – boundaries of the distribution area of the Caledonian structural complex (without the Devonian Gargždai Group); 4 – the state boundaries; 5 – the geological age of deposits exposed directly under the Hercynian structural complex: Cm – Cambrian; O_1 – Lower Ordovician; O_2 – Middle Ordovician; O_3 – Upper Ordovician; S_{ln} – Silurian, Llandovery; S_w – Silurian, Wenlock; S_{ld} – Silurian, Ludlow; S_{pr} – Silurian, Pridoli. Compiled by K. Popovs.

The same problems complicate the division of lithostratigraphical units in the Rēzekne and Pärnu RS. The Rēzekne Fm corresponds to the Rēzekne RS in the eastern part of the south-east Baltics, but the Lemsi Formation is attributed to the same RS in south-western Estonia (Paškevičius, 1997; Kleesment and Mark-Kurik, 1997a). The Pärnu Fm is attributed to the Pärnu RS in all its distribution area (Paškevičius, 1997) or to the Pärnu RS in the eastern and northern part of the south-east Baltics and as both - Rēzekne and Pärnu RS in the central and western parts of the south-east Baltic States, where the division of the two formations is problematic (Kurshs, 1975; Gailīte et al., 2000).

The depositional environment in the epeiric sea during the Rēzekne-Pärnu time was determined by river water influx from the main provenances situated north of the basin, a dominant arid climate in the sea, two tectonic barriers regulating the current directions and clastic material distribution (Kuršs and Stinkulis, 1998) and the influence of tidal processes (Tovmasyan, 2004).

The open sea lay west of the Baltic Basin and was partly separated from it by the northwest-southeast barrier - northern part of the Belarus-Mazury Anteclise (Kuršs and Stinkulis, 1998). Clayey deposits prevailed in the western part of the epeiric basin nearest to the open sea. Strong river inflow from the north lowered salinity and carried in a large amount of sandy sediments. The northern part of the eastern Baltics is therefore predominated by sandstones. It is likely that freshwater inflow did not reach the southern part of the sea, therefore dolomite and gypsum cement of a probable early origin often occurs there.

A large carbonate platform formed on and to the east of the Vilaka arches (Kuršs and Stinkulis, 1998). In the western part of the carbonate platform, sandy-clayey carbonate sedimentation dominated. The structures of the deposits presumably are characteristic of changeable water agitation. Facies of laminites with conformable bedding are also typical for these beds. Structures of clayey carbonate deposits indicate the existence of the tidal environment at least in some areas (Kuršs and Stinkulis, 1998).

Further to the east (Drissa and Liozno) deposits contain even less clastic admixture, and are represented by the clayey dolomites. The gypsum lenses and intercalations often occur in the clayey carbonate sediments. Eastwards from the Vilaka arch in the upper part of the sequence, gypsum appears and thickens to the southeast, halite even appears towards the east, so it is likely that the central part of the Moscow Syneclise was occupied by the hypersaline basin (Tihomirov, 1995; Kuršs and Stinkulis, 1998). It should be noted that the carbonate platform separated the eastern Baltic epeiric sea from the hypersaline basin of the Moscow Syneclise and in its largest part was adjacent neither to the open sea, nor the land areas (Kuršs and Stinkulis, 1998).

Features of tidal influence were noted in the Rēzekne and Pärnu fms in the eastern part of the south-east Baltic (Kuršs and Stinkulis, 1998), and identified and described in detail in the Pärnu Fm in the northern part of the study area (Tovmasyan, 2004). The latest data suggests that the Pärnu Fm is composed of a transgressive, tidally controlled estuary sequence. A fluvial, fluvial to estuary transitional zone, open estuary and tidal flat facies assemblages have been identified in the Pärnu Fm (Tovmasjana and Plinka-Bjorklunde, 2010).

The surface of the Pärnu Fm well characterises the tectonic structure of the lower part of the Hercynian structural complex (Fig. 7). The maximum depth of this surface is in the westernmost Lithuania (more than -900 m) and rises eastwards to the central Latvia (-400 to -300 m) and to the north-western Latvia. This area corresponds to the Latvian-Lithuanian Depression (Brangulis and Kaņevs, 2002), which was the area of maximum subsidence in the Devonian time in the south-east Baltic States (Brangulis et al., 1998), and it partly corresponds to the Polish-Lithuanian Depression (Paškevičius, 1997).

In the eastern Latvia there is another local and less sharply expressed subsidence area, where the surface of the Pärnu Fm lays in depth of -350 m, referred as the Latvian Saddle (Brangulis and Kaņevs, 2002). In northern Latvia and southern Estonia the surface northwards gradually gets shallower and reaches Earth surface in southern Estonia. This area is referred as the Estonian-Latvian monocline (Brangulis and Kaņevs, 2002). In south-eastern Latvia, eastern and south-eastern Lithuania there is another area, where this surface becomes shallower eastwards and south-eastwards. It is called the slope of the Belarus-Mazurian Anteclise (Paškevičius, 1997).

5.5.3. Middle Devonian

The Eifelian succession continues with the **Narva RS**. The Narva Fm corresponds to the whole volume of the Narva RS. It is divided into three parts in Latvia and Estonia – the Leivu, Vadja and Kernavė members (Kleesment and Mark-Kurik, 1997b; Gailīte et al., 2000). In Lithuania the Ledai and Kernavė Fms are united into the Narva RS (Paškevičius, 1997). The Ledai Fm corresponds to the Vadja and Leivu members in other parts of the Baltic Basin.

The Narva RS clearly differs from other Lower and Middle Devonian deposits in the Baltic Basin by its clayey and carbonate deposits. The Vadja and Leivu beds, as well as the Ledai Fm are composed of an alternation of dolomite, dolomitic marl and other clayey carbonate deposits with gypsum and anhydrite (Tänavsuu-Milkeviciene et al., 2009). The Kernavė beds are made of various clayey and carbonate deposits with sandstone interlayers in their lower part. Invertebrate fossils indicating an open marine environment are present only in the limestone of the Kernavė Member in the southern part of the Baltic Depression (Kurshs, 1992). In the northern part of the Baltic Depression, sandstones are dominant in the Kernavė Member.

A breccia lies at the base of the Vadja Member, containing clasts of both the above-mentioned clayey to carbonate deposits and older (Pärnu age) sandstones. The origin of the breccia is interpreted as being due to the slump processes (Kurshs, 1992) or the sabkha brecciation (Tänavsuu-Milkeviciene, et al. 2009).

The maximum transgression of the Eifelian basins took place during the Narva time, and reached its widest extent during the Leivu time (Kurshs, 1992). A detailed study of facies associations and the palaeogeographic reconstruction of the Narva time (Tänavsuu-Milkeviciene, et al. 2009) suggest that during the transgression, sabkha and supratidal to intertidal deposits developed on the basin margins, and subtidal carbonates in the basin centre. Subsidence across the whole basin took place by the end of this phase. The upper part of the succession is interpreted as progradational deltaic deposits. The wide influence of tidal processes is suggested for the Narva basin (Tänavsuu-Milkeviciene, et al. 2009).

The Eifelian Stage is followed by the **Aruküla RS**. The Aruküla Fm corresponds to this RS in Latvia and Estonia and the Kukliai Fm (lower part of the Upninkai Group) in Lithuania (Paškevičius, 1997). Three units are divided in the Aruküla Fm in Estonia – the Viljandi, Kureküla and Tarvastu beds (Kleesment and Mark-Kurik, 1997b). The lower part of the Aruküla RS is composed of sandstone, but the upper, thicker part is made of red siltstone of irregular structure (Kurshs, 1992). The clayey and silty deposits of the Aruküla RS are rich in carbonate inclusions of irregular shape and distribution. Their content decreases towards the west (Kurshs, 1992). In Estonia, the Viljandi beds are composed of very fine-grained sandstone with platy bedding, the Kureküla beds are made of an alternation of siltstones, sandstones and conglomerates with clay clasts, but the Tarvastu beds are rich in conglomeratic interbeds (Kleesment and Mark-Kurik, 1997b).

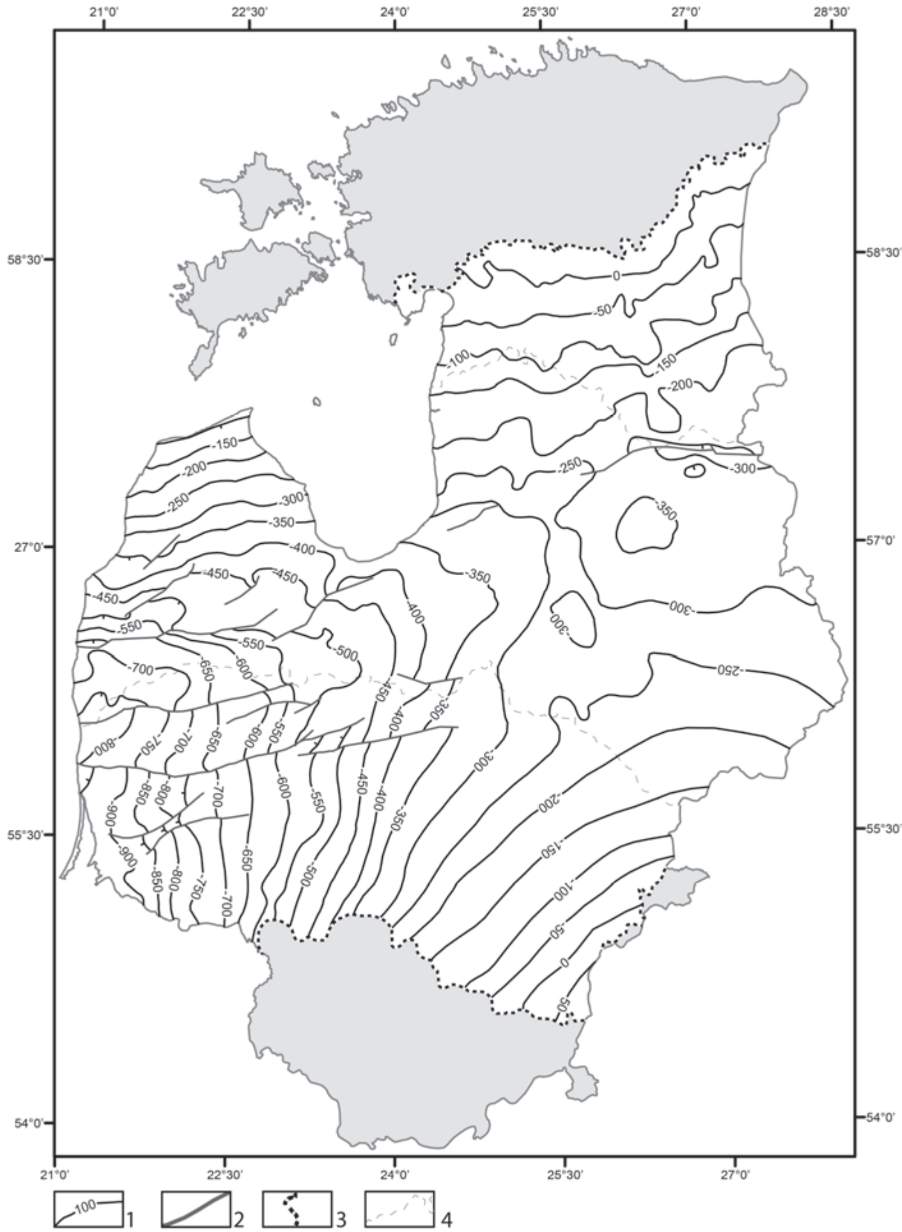

Figure 7. The Pärnu Fm surface map: 1 – The Pärnu Fm surface contour lines; 2 – faults; 3 – boundaries of the distribution area of the Pärnu Fm; 4 – the state boundaries. Compiled by K. Popovs.

The largest (central) part of the Aruküla basin has been occupied by facies of silty and sandy sediments. In the north-western part of the basin close to the provenances the sandy sediments are dominant. In later detailed sedimentological study, the siliciclastics of the Aruküla Fm (and slightly older Kernavė beds) have been interpreted as tide-dominated delta deposits (Tänavsuu-Milkeviciene et al., 2009). The facies change and measurements of the cross-strata dip azimuths indicate that the clastic material was transported into the sedimentary basin mainly from the north (Kurshs, 1992).

The Givetian Stage starts with the **Burtnieki RS**. Like the Aruküla RS, its lower part is dominated by sandstone, but the upper part by siltstones and clays. The Burtnieki Fm corresponds to the Burtnieki RS in Latvia and Estonia, and the Butkūnai Fm (upper part of the Upninkai Group) to the Burtnieki RS in Lithuania (Paškevičius, 1997). In Estonia, on the basis of lithological and mineral composition, three cyclic units are divided in the Burtnieki Fm – the Härma, Koorküla and Abava beds (Kleesment and Mark-Kurik, 1997b).

The basin of the Burtnieki time is characterised by distinct facies zonation (Kurshs, 1992). The finds of marine invertebrates in north-eastern Poland indicate that the Baltic Basin was still connected with the open sea in the south-western regions (Kurshs, 1992). The major part of the Main Devonian Field was covered by a shallow brackish-water sea with clayey to silty deposits and sands in a proportion of about 1:1 in the axial part of the Latvian-Lithuanian Depression and also eastwards from Latvia – in the Moscow Syneclise (Kurshs, 1992). These areas were separated from each other by a rather wide submeridional belt spreading across almost the whole basin from Ilmen Lake to eastern Belarus with dominant sand sedimentation.

The submarine part of the delta existed in the northern areas along the main provenances. Presumably the deltaic deposits have been preserved from post-Devonian erosion in the small area in south-eastern Estonia. Sandy deposits are dominant though clays are present as well. The existence of the deltaic zone is confirmed by the presence of the slump depressions filled by very fine clayey deposits (Kurshs, 1992). The facies zone of sandy dolomitic marls, which are quite widespread along the eastern coasts of the Rēzekne-Pärnu and Gargždai basins, presumably also developed during the Burtnieki time and are situated at the southern margin of the basin (Kurshs, 1992).

Sedimentological studies in the Veczemji outcrop reveals the strong influence of tidal processes in the deposition of the siliciclastics of the Burtnieki Fm (Tovmasjana et al., 2011).

In western, central and south-eastern Latvia, the Gauja Fm as a whole is attributed to the Gauja RS. The Gauja Fm in Latvia is represented by fine and medium grained sandstones, siltstones and clays. Sandy deposits dominate in the lower part, but siltstones and clays - in the upper part of the formation. In north-eastern Latvia both Gauja RS are subdivided into two formations – the Sietiņi Fm in the lower part and the Lode Fm in the upper part of the Gauja RS. The Sietiņi Fm is composed of light-grey sandstone which clearly differs from the yellow to red sandy deposits of the Gauja Fm. The Lode Fm in general is similar to the clayey and silty deposits of the upper part of the Gauja Fm, but it contains lenticular bodies of yellowish-grey very fine clay which fill local slump depressions (Kurshs, 1975; 1992).

In Estonia, the Gauja RS is represented by one formation (Gauja Fm) divided in two members – the Sietiņi and the Lode Member (Kleesment and Mark-Kurik, 1997b). The Sietiņi Member is composed of light-coloured sandstone, which changes into variegated siltstone only in the topmost part, but the Lode Member is made of light-coloured sandstone in the lower part and clayey deposits in the upper part (Kleesment and Mark-Kurik, 1997b).

In Lithuania the Gauja RS and overlaying Amata RS are unified in the Šventoji RS, and one – the Šventoji Fm, has been divided (Paškevičius, 1997).

The deposits of the Gauja, Sietiņi and Lode fms formed during the Gauja time. V. Kuršs (Kurshs, 1992) suggests that a new transgression of the Devonian sea started in the Gauja time, when sediments accumulated on the eroded surface of the Burtnieki Formation. This time, like the previous Burtnieki time, was characterised by distinct facies zonation of the basin.

V. Kuršs (Kurshs, 1992) has suggested that most of the Main Devonian Field was covered by a shallow brackish-water sea. Clayey-silty deposits and sand in an almost similar proportion accumulated in the axial part of the Latvian-Lithuanian Depression (south-western Latvia and north-western Lithuania), which was situated close to the open sea. In addition, similar deposits formed westwards from Latvia - in the Moscow Syneclise. These areas were separated from each other by a rather wide submeridional belt dominated by sand and spreading across almost the whole basin from Ilmen Lake to eastern Belarus. The deltaic zone situated in the northern part of the palaeobasin during the Gauja time likely prograded southwards if compared with the previous Burtnieki time – up to the present area of north-eastern Latvia (Kurshs, 1992).

In a recent study (Pontén and Plink-Björklund, 2007) the Gauja RS has been attributed to a subaqueous to subaerial tide-influenced delta plain and front. It has been suggested that a change from progradation to aggradation during the Gauja time took place and it was associated with a vertical decrease in tidal influence and a decrease in coarse-grained sediment input.

The slump depressions, up to tens of metres wide and deep, are documented in detail in the Lode Fm in the Liepa clay pit, and these features indicate the delta front settings during the end of the Gauja time in north-eastern Latvia (Kurshs, 1992; Blāķe, 2010).

The **Amata RS** corresponds to the uppermost part of the Lower- to Middle Devonian siliciclastic sequence. One formation – the Amata Fm, is divided in this regional stage in Latvia and Estonia (Kurshs, 1992; Kleesment and Mark-Kurik, 1997b). This formation is composed of yellowish and light grey fine grained sandstone, as well as reddish brown siltstone and clay. In Lithuania their age-equivalent is the upper part of the Šventoji RS and correspondingly the Šventoji Fm (Paškevičius, 1997).

According to V. Kuršs (Kurshs, 1992), the Amata time, like the previous Gauja time was characterised by a transgression of the basin. The transgression was wider than previously, and the deposits of the Amata Fm in the north-eastern Baltic with a stratigraphic gap cover older beds. .

V. Kuršs has divided the two facies zones of the basin of the Amata time. Silts and sands accumulated in shallow water in the axial part of the Latvian-Lithuanian Depression (south-western Latvia and north-western Lithuania), as well as in the Moscow Syneclise. Northwards the water was still shallower and sandy deposits prevailed considerably there (Kurshs, 1992).

In recent studies (Pontén and Plink-Björklund, 2009) the conclusion is made that the Amata Fm was deposited in tide-dominated estuaries and records depositional environments such as fluvial channels and outer-estuarine tidal bars. They suggest that the estuarine tidal bars have such typical features as preserved topsets, evidence of landward palaeocurrent directions, well to very-well-sorted, very fine- or fine-grained sandstones and overall transgressive stacking.

5.5.4. Upper Devonian

The Upper Devonian deposits are widespread and well-exposed in the south-eastern Baltic States, especially in Latvia and Lithuania. Both the Frasnian and Famennian Stages are present.

5.5.4.1. Frasnian Stage

The lower part of the **Pļaviņas RS** (Koknese Mb and correlated stratigraphical units) is composed of dolomitic marl, clay, sandstone and dolomite, but the other parts of section are dominated by dolomites (Brangulis et al., 1998; Kajak, 1997; Paškevičius, 1997).

The Pļaviņas time corresponds to significant changes in the sedimentary environment of the Baltic Basin. Siliciclastic sedimentation, which dominated from the beginning of the Devonian period until the end of the Amata time (likely to the end of the Middle Devonian) was changed by the accumulation of carbonate and clayey deposits. An epeiric sea still existed in the Baltic Basin, but starting from the Pļaviņas time it was open to the east. It is evidenced by invertebrate fossil-rich limestones present in north-easternmost Latvia and south-eastern Estonia, as well as further east in Russia. In central Latvia and the central part of northern Lithuania fossil-rich carbonate deposits are still dominant but are completely dolomitized. In western Latvia, north-western and western Lithuania clayey dolomites, dolomitic marls and clays are dominant, and even lenses and layers of gypsum appear (Sorokin, 1978; Brangulis et al., 1998).

Most of the Devonian carbonate deposits and carbonate admixtures in the siliciclastic deposits in the south-east Baltic States are composed of dolomite. It has been suggested that the dolomitization of the carbonate deposits have taken place from Devonian sea water, which served as a source of magnesium. Sulphate precipitation and the removal from the solution, as well as other still unknown modifications of sea water composition are proposed as the reasons for the initiation of the dolomitization processes (Stinkulis, 2008).

The **Dubnik (Dubniki) RS** is represented by the Dubniki Fm in south-eastern Estonia and north-eastern Latvia, by the Salaspils Fm in central and western Latvia and by the Pasvalys beds (lower part of the Tatula Group) in Lithuania (Gailīte et al., 2000; Kajak, 1997; Paškevičius, 1997).

The Dubnik time was marked by a considerable regression of the basin (not only in the Baltic, but in all of the East-European Craton), when it became shallower, and the sedimentary regime was largely regulated by the bottom-structures - highs and arches (Sorokin, 1978). These positive structures hindered an inflow of normal-salinity water from the Moscow Syneclise, therefore the salinity of water increased under the arid climate conditions. It caused the formation of penecontemporaneous dolostones and gypsum, as well as creating an unfavourable environment for organisms (Sorokin, 1978).

In eastern Latvia and southernmost Estonia clayey dolomites and dolomitic marls are dominant. The role of dolomitic marls and amount of gypsum increases westwards, but in the western part of Lithuania gypsum together with carbonate deposits are present. In northern Latvia an increased amount of clay is noted (Sorokin, 1978).

It is important to note that gypsum deposits are found in several local areas like in the vicinity of Salaspils, Saurieši and Saulkalne (east of Riga), Skaistkalne and Mālpils-Jūdaži. Gypsum-rich deposits formed in a hypersaline lagoon and/or sabkha environment. Geological sections of gypsum-rich deposits of the Dubnik RS are of rhythmically changeable composition (Brangulis et al., 1998).

The **Daugava RS** like the Pļaviņas RS is dominated by dolomites. The Oliņkalns Member (lower) and Kranciems Member (upper) and their correlative units are dominated by dolomites, but the Selgas Member (middle) and its age-equivalents by the dolomitic marls, clays and clayey dolomites (Brangulis et al., 1998).

The high content of carbonates in the Daugava RS is related to the sedimentary environment of the palaeobasin – the wide transgression of the epeiric sea, salinity of water close to normal seawater, as well as a small amount of the siliciclastic input. Lateral facies changes are gradual which also indicate transgression during the Daugava time. The facies zonation generally is similar to that of the Pļaviņas time: fossiliferous limestones dominate in north-eastern Latvia and neighbouring areas, in central and eastern Latvia dolomites are present with a rich assemblage of invertebrate fossils, but in western Latvia and north-western Lithuania an alternation of dolomites, dolomitc marls and clays (Brangulis et al., 1998). An admixture of gypsum is noted in the Daugava RS in north-western Lithuania and its content increases southwards (Sorokin, 1978).

The Katleši RS in Latvia and Lithuania is represented by the Katleši Formation (Sorokin, 1981; Paškevičius, 1997). In Estonia this unit and younger pre-Quaternary deposits have not been found. In Latvia the Katleši Fm is subdivided into 3 members - the Ikšķile, Liepna and Kuprava. The Ikšķile member comprises one, and the Liepna member - two cycles. Each cycle is composed of relatively thin (1-2 m) sandstone or dolomite beds in the lower part and thick carbonate clay or dolomitic marl beds (3-9 m) in the upper part. The upper one, the Kuprava Mb, occurs only in local areas along the southern part of the Riga-Pskow Step. The Kuprava Mb is composed of clays with interbeds of clayey siltstones and dolomitic marls (Sorokin, 1978; 1981). Dolocrete, up to 1 m thick, has been documented in the Kuprava Mb in the Kuprava clay pit (Stinkulis and Spruženiece, 2011).

In south-western Latvia and Lithuania, the Katleši Fm is likely represented only by its lower part composed of sandy to silty and clayey dolomite alternating with silty dolomitic marls and dolomitic clays (Sorokin, 1981).

The facies changes of the Katleši Fm are not distinct. In the northern part of its distribution area this formation becomes more clayey and sandy. In central Latvia there are more dolomite and dolomitic marl interbeds, but in south-western Latvia and northern Lithuania interlayers of gypsum appear (Sorokin, 1981).

The Pamūšis RS is represented by the Ogre Fm in Latvia and Pamūšis Fm in Lithuania (Sorokin, 1981; Paškevičius, 1997). In Latvia the Ogre Fm is subdivided into three members. The Lielvārde and Rembate Mbs are composed of sandstones with carbonate cement, silty clays and dolomitic marls, but the Suntaži Mb is represented by variegated clays and dolomitic marls (Sorokin, 1981). The Pamūšis Fm is composed of marls with interlayers of gypsum, clay and siltstone in north-western Lithuania and alternation of sandstone, clay, marl and dolomite in the central part of northern Lithuania (Narbutas, 1981a).

The beginning of the Ogre time was marked by an essential restructuring of facies zonality and palaeogeography of the basin (Sorokin, 1978; 1981). Contrary to the Daugava-Katleši times, when the basin transgressed from the east, during the Ogre time it likely advanced from the southwest (Sorokin, 1978). The Ogre basin differed from other Frasnian basins by a large inflow of sand (Brangulis et al., 1998). The **Stipinai RS** in Latvia and Lithuania is represented by the Stipinai Fm, which in Latvia is divided in the Imula and Bauska mbs (Paškevičius, 1997; Gailīte et al., 2000). These deposits are present in the Latvian-Lithuanian depression (south-western Latvia and north-western Lithuania), and occur in eastern Latvia only as several "island-like" erosional remnants (Brangulis et al., 1998). The Imula Mb is composed of alternating dolomite, clayey dolomite and dolomitic marl, and occasionally clay. In the northern part of its distribution area, sandstone and siltstone interlayers are present in the lower part of the section. The Bauska Mb is made mostly of dolomite, often fossiliferous. In the upper part of this member and towards the northern part of its distribution area, the amount of clay increases (Sorokin, 1981; Brangulis et al., 1998).

The Stipinai time corresponds to the transgression of the sea which was open to the south-west. Carbonate sedimentation dominated, especially when the Bauska Member formed. Close to the central part of the basin (in Lithuania and south-western Latvia), siliciclastic input was insignificant, and the salinity of water was close to normal seawater, therefore carbonate sediments accumulated and various organisms developed (Brangulis et al., 1998). The clay and sand admixture was higher close to the seacoast (northwards), and clayey-silty material accumulated together with carbonate sediments (Brangulis et al., 1998). The **Amula RS** is present only in the Latvian-Lithuanian depression. In Lithuania and Latvia this regional stage is represented by the Pakruojis and Amula Fms, correspondingly (Paškevičius, 1997). The Pakruojis Fm in the north-western part of its distribution area is composed of dolomitic marls with an admixture of gypsum and in the north-eastern part of dolomites, marls, clays, siltstones and micaceous sandstones (Narbutas, 1981b). The Amula Fm in the northern part of its distribution area is composed of cyclically alternating sandstones, siltstones and silty dolomites with variegated clays, clayey siltstones, dolomitic marls and platy dolomites. Southwards the sandstones changes into silty and sandy dolomites. In westernmost Latvia, layers of gypsum-rich dolomite and gypsum appear in this formation. Lithology and sedimentary structures indicate a lagoon-like environment (Sorokin, 1981).

5.5.4.2. Famennian Stage

The Famennian Stage is present only in south-western Latvia and north-western Lithuania. It is composed of laterally and vertically variable deposits - sandstones, dolostones, dolomitic marls, clays, siltstones and limestones. The Famennian basin was situated in the Latvian-Lithuanian Depression, which in the west and southwest periodically connected with the open sea (the same as at the end of the Frasnian time). At the times of maximum transgressions it probably also contacted with the sea of Middle Russia through the Pripyat Deep (Savaitova, 1977). Generally, the role of marine fossiliferous limestones increases towards the south and southwest, but the dolomitization degree of deposits, as well as the admixture of sand and clay - towards north. The northern areas, like in previous Devonian times, served as the main provenances.

The **Kruoja RS** in Lithuania is represented by the Kruoja Fm and composed of laminated and thick-bedded clayey dolomites and rarer limestones. The **Šiauliai RS** in Lithuania has a corresponding Šiauliai Fm made of dolomitic marls, siltstone, clay and dolomite (Paškevičius, 1997). In Latvia one unit, the **Eleja Fm,** is attributed to this regional stage. It is composed of dolomitic marls, dolomites and clays with interlayers of sandstone and siltstone. Three members are distinguished in the Eleja Fm in Latvia. The Purviņi Mb consists of clay, clayey siltstone and dolomitic marl, the Cimmermaņi Mb is composed of dolomitic marl, clayey siltstone and clay with interlayers of dolostone, but the Sesava Mb is made of dolomitic marl and crystalline dolomite (Gailīte et al., 2000). In the Kruoja and Šiauliai regional stages, the content of clay increases towards the palaeocoastline (to the north), but the carbonate amount southwards, to the central part of the basin (Brangulis et al., 1998). Marine to lagoonal settings existed during these times (Savaitova, 1977).

The Joniškis Fm in Latvia and Lithuania corresponds to the **Joniškis RS** (Paškevičius, 1997). Fossiliferous limestone is dominant in these beds in Lithuania and southwesternmost Latvia, but in the northern part of the distribution area (southern Latvia) limestones gradually change into dolomites and the admixture of clayey and sandy material slightly increases (Savaitova, 1977). Sedimentological and palaeontological data provide evidence of open marine settings in wide areas during the Joniškis time.

One unit, the Kuršiai (Kursa) Fm, is divided in the **Kuršiai (Kursa) RS** both in Lithuania and Latvia (Paškevičius, 1997, Gailīte et al., 2000). The Kuršiai Fm is also dominated by fossiliferos carbonate deposits represented mostly by limestones in north-western Lithuania and by dolomites in south-western Latvia. In northern and north-eastern parts of the unit distribution area sandy to silty dolomites, and at the northernmost areas sandstones, siltstones and clays are present (Zheiba and Savaitova, 1981). A marine environment is supposed to have existed during this time in the central part of the basin, but more restricted basinal settings with fluvial influence dominated closer to the coastline in the north (Savaitova, 1977).

The **Akmene RS** in Lithuania and Latvia is represented by the Akmene Fm (Paškevičius, 1997; Gailīte et al., 2000). In north-western Lithuania (except the north-westernmost corner) fossiliferous limestone and dolomite predominate. In the northern and western parts of the distribution area of this formation, dolomites with sand admixture, dolomitic marls and clays are present, but in the north-eastern areas sandstones and clays with some dolomite interlayers (Savaitova, 1977). More widely distributed open marine settings have been supposed for this time in comparison to the Kuršiai time, however, towards the north and especially the north-east, the influence of clastic material from the continent increased (Savaitova, 1977).

The **Mūri RS** is represented by one unit, the Mūri Fm, both in Lithuania and Latvia (Zheiba and Savaitova, 1981). It is one of the sandiest Famennian units. In most of its distribution area there are poorly cemented, in places, cross-stratified sandstones, but siltstones and clays are present in a smaller amount (Brangulis et al*.,* 1998). The Mūri succession is composed of clayey and sandy dolomitized limestones with rare interlayers of marls and sandstones only in north-westernmost Lithuania (Zheiba and Savaitova, 1981). A marine environment dominated during the Mūri time in the south-western areas, but a considerable inflow of freshwater and sand took place in the northern part of the palaeobasin.

The **Švėtė RS** is divided into two formations (Tērvete and Sniķere fms) in Latvia (Zheiba and Savaitova, 1981), and one formation (Švėtė Fm) in Lithuania (Zheiba and Savaitova, 1981; Paškevičius, 1997). In Latvia the **Tērvete Fm** is composed of sandstone, siltstone and clay with vertebrate fossils, but the **Sniķere Fm,** by dolomites with invertebrate remains, sandstones and siltstones with carbonate cement (Zheiba and Savaitova, 1981). In Lithuania the **Švėtė Fm** is made of an alternation of sandstones, siltstones and clays in the lower part and an alternation of sandstones, sandy dolomites, dolomitic marls and siltstones in the upper part. In the south-western part of its distribution area, the succession of the Švėtė Fm is dominated by sandy dolomite with interlayers of nodular limestones in the lower part (Zheiba and Savaitova, 1981).

It's necessary to note that L. Savvaitova proposes the name Spārnene RS for the Mūri and Tērvete Fm, and the lower part of the Švėtė Fm (Lukševičs et al., 1999). This proposal was also supported later (Vasiļkova et al*.*, 2012).

The distribution of the Tērvete Fm and the presumably age-equivalent part of the Švėtė Fm is irregular, and these deposits are not present in south-westernmost Latvia and north-westernmost Lithuania (according to Savaitova, 1977). However, it can be supposed that the open marine environment was not characteristic for this time (Savaitova, 1977).

A recent study of the deposits of the Tērvete Fm in the Klūnas outcrop (eastern part of the distribution area of this formation) allows the conclusion that these sandy to clayey deposits were formed under the influence of fluvial and tidal processes in the shallow-water environment, at least partly as the infilling of erosional channels, thus evidencing deltaic or estuarine settings (Vasiļkova et al., 2012).

During the time when the Sniķere Fm and the upper part of the Švėtė Fm formed, the open sea environment renewed, first in the south-western part of the basin, and during the middle of this time - spread in most of the present distribution area of these deposits. At the end of this time such settings almost diminished. All during this time interval (especially in the beginning and the end) there was a considerable inflow of sandy and clayey material from the north (Savaitova, 1977).

The Žagarė RS in Latvia and Lithuania is represented by Žagarė Fm (Paškevičius, 1997). It is composed of fosiliferous dolomites in north-western Lithuania and south-westernmost Latvia, sandy dolomites (in the lower part of the succession) and fossiliferous dolomites (in the upper part of the succession) in a wide zone along the present boundary of Latvia and Lithuania and carbonate-rich sandy to clayey deposits in the north. During the Žagarė time the open marine environment was dominant, however in the northern part of the basin, a considerable inflow of sand and clay is reported (Savaitova, 1977).

The **Ketleri RS** contains one formation, the Ketleri Fm (Paškevičius, 1997; Gailīte et al., 2000). In Latvia it is divided into three parts: the Nīgrande, Pavāri and Varkaļi members. The Nīgrande Member is made of clay, clayey siltstone and dolomitic marl, but the Varkaļi Member and the Pavāri Member are composed of dolomitic marl, siltstone, clay and sandstone, and are rich in vertebrate fossils (Gailīte et al., 2000).

The Pavāri Member was studied in detail in the Pavāri site (north-eastern part of the distribution area of the Ketleri Fm) and the first fossil tetrapods in Latvia were documented there together with numerous fish remains (Ahlberg *et al.,* 1994). Later it was suggested that, possibly, deposits of the Pavāri locality formed in a low-tidal terrigenous shelf environment between low islands where a shallow channel might have been formed in tidal processes (Lukševičs and Zupiņš, 2004).

In Lithuania, the Ketleri Fm is composed of clayey dolomites with interlayers of clays and siltstones in the lower part and sandstones with interlayers of clays, siltstones and dolomitic marls in the upper part. Various facies in the basin can be divided (Жейба & Savaitova, 1981). The deposits of the Ketleri Fm in the present area of Latvia and Lithuania possibly accumulated in the shallow lagoon-like basin with a considerable influx of siliciclastic material (Brangulis et al*.,* 1998).

The Šķervelis Fm is the only lithostratigraphical unit in the uppermost part of the Devonian succession, **the Šķervelis RS**, in the south-east Baltic States (Paškevičius, 1997). In Latvia it is divided in two parts, the Gobdziņas un Nīkāce members. The Gobdziņas Member is made of cross-stratified sandstone with irregular dolomite, rarer chert cement, but the Nīkrāce Member is composed mostly of dolomite with a chert admixture (Gailīte et al*.,* 2000). In Lithuania, the Šķervelis Fm contains more carbonate material and also a clay admixture (Brangulis et al*.,* 1998). The deposits of the Gobdziņas Member were likely to have formed in a shallow sea with considerable clastic inflow from the north. In the last decade, the Nīkrāce Member has been interpreted as a thick dolocrete – carbonate crust formed in a desert or similar environment during the regression of the sea basin (Stinkulis, 2004).

5.6. Carboniferous

Carboniferous deposits are distributed in a relatively small area in north-western Lithuania and south-western Latvia. Their maximum thickness is 112.5 m (Paškevičius, 1997). The division of the Carboniferous system in the south-east Baltic States (Fig. 8)

SERIES	STAGE	CONODONT BIOZONES	LITHOSTRATI-GRAPHIC UNITS SW LATVIA, NW LITHUANIA
LOWER CARB.	TOURNAISSIAN	*P. variabilis*	NĪCA Fm.
		P. crassus	PAPLAKA Fm.
			LĒTĪŽA Fm.

Figure 8. Stratigraphic chart of the Carboniferous deposits of Lithuania and Latvia (based on Stinkulis, 2004 for Latvia and Paškevičius, 1997 for Lithuania).

is based only on rare vertebrate fossils (Ljarskaja et al., 1981; Paškevičius, 1997). According to present opinion, the Carboniferous deposits present in the south-east Baltic States are attributed to the Lower Mississippian Subseries, Tournaisian Stage (Paškevičius, 1997; International Stratigraphic Chart, 2010).

Three lithostratigraphical units are divided in the Tournaisian of the south-east Baltic States: the Lētīža, Paplaka and Nīca Fms (Paškevičius, 1997; Gailīte et al., 2000).

The **Lētīža Fm** is composed of alternating sandstones, clays, clayey siltstones and dolomitic marls. It is likely that the deposits of this formation formed in a shallow, partly restricted basin. The **Paplaka Fm** consists of dolomitic marls, clays, dolomites and sandstones. The **Nīca Fm** is represented only by poorly cemented, well-sorted, yellowish grey, less frequently red sandstones. Their accumulation is supposed to have taken place in a shallow basin with an intense supply of siliciclastic material (Brangulis et al., 1998; Paškevičius, 1997; Savaitova and Zheiba, 1981). Facies zonation and the sedimentary environment of the Carboniferous deposits have not been studied in detail yet due to poor exposures and drillcore material.

5.7. Permian

Permian deposits are widely distributed in western and southern Lithuania, as well as in south-western Latvia. Their thickness in Latvia reaches 35 m in Latvia and 100 m in Lithuania, but increases to 300 m south-westwards in the Kaliningrad district (Russia) and even to 600 m further to the south-west in Poland (Kurshs and Savaitova, 1986; Paškevičius, 1997).

Two regional stages, Verra and Stassfurt RS (Fig. 9), corresponding to analogues in north-western Europe are divided in the Permian of the south-east Baltic States (Paškevičius, 1997). Both these regional stages are attributed to the Zechstein and to the previously used Uffian (upper part) and Kazanian stages (Paškevičius, 1997). According to the present stratigraphic subdivision (International Stratigraphic Chart, 2010; Menning et al., 2006) these units belong either to the Lopingian Series (Upper Permian) or to the Guadalupian Series (Middle Permian). Both regional stages are present in Lithuania, but only a part of the Verra RS occurs in Latvia (Paškevičius, 1997). In the Kaliningrad district (Russia) younger deposits of the Leine RS are also present.

The **Verra RS** is subdivided into 4 formations, the Kalvarija, Sasnava, Naujoji Akmenė and Prieglius Fm. The Kalvarija Fm is present only in southern Lithuania and composed of conglomerate, gravelstone and sandstone with carbonate, clay, gypsum and pyrite (Suveizdis, 1994a; Paškevičius, 1997). These beds are supposed to be basal conglomerates of the transgressive Zechsteinian sea (Paškevičius, 1997). The Sasnava Fm is also present in southern Lithuania. The formation is composed of dark-grey bituminous clay, siltstone and sandstone. Northwards dolomite interlayers appear. The Sasnava Fm yields sulphide mineralisation and can be correlated with the age-equivalents of similar composition in Western Europe (Suveizdis, 1994a).

The Naujoji Akmenė Fm corresponds to the maximum expansion of the Permian basins, and these deposits are the most widespread of the Permian of the south-east Baltic States. This formation is composed of conglomerate, sand, marl and clayey limestone in its lower part, as well as limestone and dolomitic limestone in the middle and upper part (Paškevičius, 1997).

The Naujoji Akmenė Fm is the only Permian unit present in Latvia. It consists of sandy limestone (Sātiņi Member) and clayey limestone (Auce Member) in its lower part, but the dominant part of the succession is represented by various limestones. The Kūmas Member is composed of earthy limestone with interlayers and nodules (»loafs«) of porcelain-like limestone. The Alši Member is made of biodetrital limestone and skeletal limestone, but the upper one, the Pampāļi Member is represented by dolomitised limestone and ooidal dolostone (Kurshs and Savaitova, 1986; Gailīte et al., 2000).

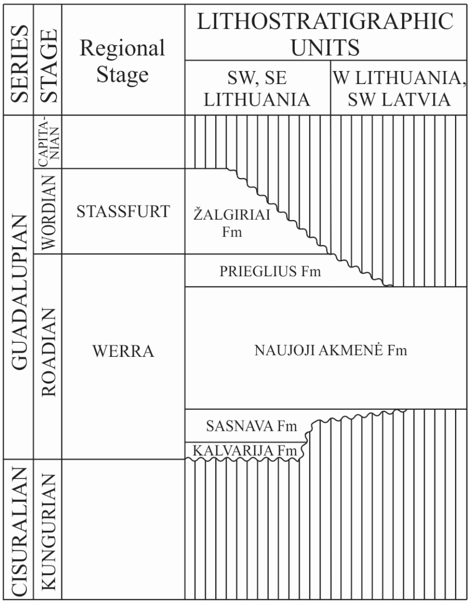

Figure 9. Stratigraphic chart of the Permian succession of Lithuania and Latvia (based on Paškevičius, 1997 for Lithuania and Stinkulis, 2004 for Latvia).

During the Naujoji Akmenė time, a large bow-like barrier reef stretched from western to central and then to southern Lithuania, as well as further to the south-easternmost corner of the Kaliningrad district and north-easternmost Poland (Suveizdis, 1994a).

The Prieglius Fm is distributed in a much smaller area than the Naujoji Akmenė Fm, only in southern Lithuania and further to the Kaliningrad district. In Lithuania it is dominated by anhydrite and gypsum, but in its south-western part rock-salt also appears. The thickness and distribution area of rock-salt increases in the Kaliningrad district and even potassium salt appears there. The Prieglius Fm is interpreted to have been formed in regressive lagoonal settings, which followed the transgression of the sea basin during the Naujoji Akmenė time (Paškevičius, 1997).

The **Stassfurt RS** is distributed in south-western Lithuania in a significantly smaller area than the Verra RS. It is subdivided in two formations: the Žalgiriai Fm representing the transgressive development of the basin and composed of carbonate deposits, and the Aistmarės Fm corresponding to the regression of the basin and is composed of sulphate and chloride deposits. Only the Žalgiriai Fm represents the Stassfurt RS in Lithuania and it consists of limestone and dolomite, often with an admixture of bituminous material (Paškevičius, 1997).

Both these regional stages and also the Leine RS present only in the Kaliningrad district correspond to the cyclic development of the Polish-Lithuanian depression. Each regional stage is a cycle starting with transgression and carbonate sedimentation and ending with regression and the precipitation of evaporites (Suveizdis, 1994a).

6. Mesozoic succession

6.1. Triassic

Triassic deposits occur in a wide area from north-western to south-western Lithuania and are also present in south-western Latvia and the adjacent area of the Baltic sea. Their thickness reaches more than 200 m in western and south-western Lithuania and decreases to the south-east, east and north (Suveizdis, 1994b). In Latvia the thickness of the Triassic deposits changes from 1-5 m in the northern and north-eastern parts of the distribution area and increases to the south and south-west to 30-74 m (Gavrilova, 1979a). The thickness of the Triassic succession increases south-westwards in the Kaliningrad district to 400 m and in north-eastern Poland to 500 m (Paškevičius, 1997).

The Triassic deposits in the south-east Baltic States are attributed to the Lower Triassic Series, Induan to Olenekian stages (Suveizdis, 1994b; Paškevičius, 1997; Šimkevičius, 2004). They are subdivided in the Nemunas, Palanga, Tauragė and Šarkuva formations. An exception is the youngest part of the Triassic in the south-eastern Baltic States, the Nida Fm, attributed either to the Lower Triassic (Suveizdis, 1994b; Šimkevičius, 2004) or to the Upper Triassic, Norian to Rhaetian stages (Paškevičius, 1997; Šliaupa and Čyžienė, 2000).

The Induan Stage is represented by the **Purmaliai Group** divided into 3 formations: Nemunas, Palanga and Tauragė Fms (Fig. 10). All these formations are present in Lithuania, but in Latvia only the lowermost part of the section, the Nemunas Fm, occurs (Paškevičius, 1997).

The Nemunas Fm, up to 131 m thick, is composed of carbonate-rich smectite-illite clay, argillite, siltstone and marl. The deposits of this formation contain inclusions of gypsum and anhydrite in places where it directly covers the evaporites of the Permian Prieglius Fm (Paškevičius, 1997). The Nemunas Fm is the only part of the Triassic section present in Latvia. There it is composed of smectite-illite clay with interlayers of siltstone and sand. The carbonate content in clays is changeable, and in places it exceeds 15% in the lower part of the formation (Brangulis et al., 1998).

Younger Triassic deposits in the south-east Baltics are present only in Lithuania. The Palanga Fm is also composed of carbonate-rich clays dominated by smectite and mixed-layered minerals, argillite and siltstones. Its thickness changes from some metres to 102 m. In the southern part of their distribution area, the deposits of this formation contain inclusions of gypsum. Clayey deposits in places contain intercalations of ooidal limestones and marls in the south-western part of their distribution area, and sand and sandstone beds in the south-eastern part of their distribution area (Paškevičius, 1997).

The Tauragė Fm is made of clayey carbonate deposits, up to 58 m thick (Suveizdis, 1994b). In western Lithuania the formation is composed of marl with clay, siltstone, limestone and sandstone interlayers, but in south-eastern Lithuania is made of clay, marl, ooidal limestone and sandstone with ooids (Paškevičius, 1997).

The Olenekian Stage is represented by the **Nadruva Group.** In south-western Lithuania the Šarkuva Fm corresponds to this unit. It is composed of dolomitic illite-smectite clay, siltstone, sand, sandstone and conglomerate. Conglomerate or sandy to silty beds lie at the foot of the formation. The thickness of this formation reaches 45 m in south-eastern Lithuania (Paškevičius, 1997).

The Induan Stage is represented by the **Purmaliai Group** divided into 3 formations: Nemunas, Palanga and Tauragė Fms. All these formations are present in Lithuania, but in Latvia only the lowermost part of the section, the Nemunas Fm, occurs (Paškevičius, 1997).

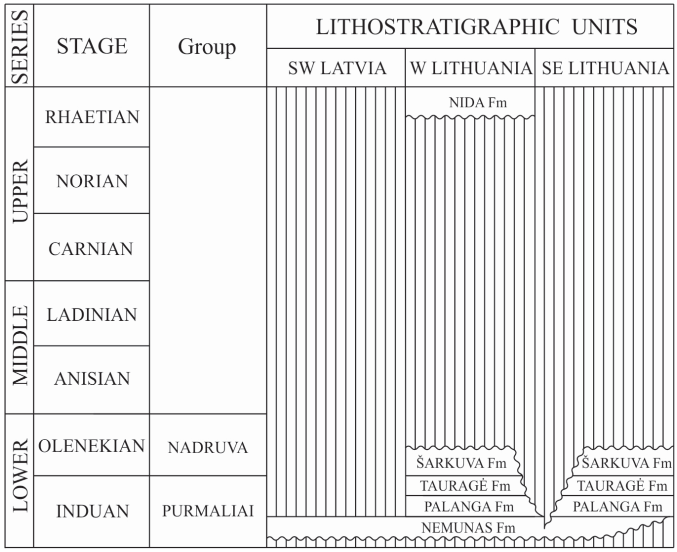

Figure 10. Stratigraphic chart of the Triassic succession of Lithuania and Latvia (based on Paškevičius, 1997 for Lithuania and Stinkulis, 2004 for Latvia).

The Nida Fm, the age of which is still being discussed (see above), is present only in south-westernmost Lithuania and is composed of siltstone, illite-kaolinite clay with sand intercalations, pyrite inclusions and wood remains. Its thickness is up to 7 m (Paškevičius, 1997) or up to 15 m (Suveizdis, 1994b). The composition of deposits points to their accumulation in a humid climate environment different from the arid climate, which most likely dominated in the early Triassic (Paškevičius, 1997).

The Triassic deposits in the south-east Baltics formed in a closed continental basin (Suveizdis, 1994b), which was most likely connected to the sea westwards and southwards (Paškevičius, 1997). The deposits of the Nida Fm represent weathering crust material (Suveizdis, 1994b).

6.2. Jurassic

The Jurassic succession (Fig. 11), like the Triassic and Permian deposits, formed in the Polish-Lithuanian Depression and occurs in western and south-western Lithuania, and in local areas in south-western Latvia (Paškevičius, 1997). In Lithuania the Lower and Middle Jurassic is represented by terrestrial and transitional (terrestrial to marine) deposits, and the Middle Jurassic (starting from the Middle Callovian) to Upper Jurassic is composed of marine deposits (Grigelis, 1994a; Paškevičius, 1997). The total thickness of the Jurassic deposits in Lithuania is up to 120 m. The deposits thin out northwards and eastwards, but their thickness increases to 240 m south-westwards outside the area of Lithuania, at the boundary between Poland and the Kaliningrad District (Russia) (Paškevičius, 1997). The Jurassic succession, up to 25 m thick, represented by Callovian and probably also Oxfordian deposits occurs in south-western Latvia (Gavrilova, 1979b, Brangulis et al., 1998).

6.2.1. Lower Jurassic

The Lower Jurassic succession occurs in south-western Lithuania and is represented by the Jotvingiai Group (Pliensbachian to Toarcian) (Šimkevičius, 2004). Its lower part (Neringa Fm) is composed of sandstone and clay with a coaly admixture and the inclusion of wood remains (Paškevičius, 1997). The thickness of the Neringa Fm reaches 33 m (Grigelis, 1994a). The upper part of the Jotvingiai Group (Lava Fm) is made of non-carbonate clay, siltstone with sand interlayers and intercalations, pyrite and charred wood inclusions (Paškevičius, 1997). The thickness of the Lava Fm is up to 45 m. The Lower Jurassic deposits are interpreted to have been formed in terrestrial, probably restricted lagoonal environment (Grigelis, 1994a).

6.2.2. Middle Jurassic

The lower part of the Middle Jurassic succession is represented by terrestrial deposits which are attributed to the Bajocian, Bathonian and Lower Callovian and unified into the Skalviai Group (Paškevičius, 1997; Šimkevičius, 2004). This group is subdivided into Įsrutis, Liepona and Papilė Fms, most likely with stratigraphic gaps in between (Paškevičius, 1997; Šimkevičius, 2004).

The Įsrutis Fm is present only in local depressions, like at Nida and Kybartai, however it has a considerable thickness, 31-89 m. The lower part of the formation is represented by clay, rich in coal, with the middle part composed of coal-rich and clayey sand, but the upper part made of silty clay (Paškevičius, 1997). It is suggested that these deposits were formed in terrestrial settings, in depressions of tectonic origin (Paškevičius, 1997).

The Liepona Fm in distributed in south-western Lithuania and composed of coal-rich clays, siltstones and sands with pyrite concretions and interlayers of coal (Paškevičius, 1997). Its thickness reaches 70 m (Grigelis, 1994a).

The Papilė Fm occurs in isolated areas in north-western Lithuania and south-western Latvia. It is represented by sand and clay, in places rich in pyrite concretions and charred wood (Paškevičius, 1997). In south-western Latvia, the Papilė Fm is dominated by quartz sand and represented also by kaolinite clay and brown coal. The composition and sedimentary structures of deposits allow it to be suggested that their accumulation occurred in a terrestrial, most likely fluvial environment. The presence of plant remains and the absence of marine invertebrate fossils support this conclusion (Brangulis et al., 1998). The thickness of this formation reaches 30 m in Lithuania (Grigelis, 1994a) and at least 13 m (in exposure at the Dzelda River bank) in Latvia.

Starting from the Middle Callovian, due to the presence of marine invertebrates, the Jurassic succession is divided into ammonite and foraminiferal zones (Paškevičius, 1997). Therefore, it is possible to better link the lithostratigraphic units with the chronostratigraphic chart.

The Papartinė Fm is attributed to the Middle Callovian and it starts a succession of supposed marine Jurassic deposits. In Lithuania this formation is up to 20 m thick and is composed of marine deposits like sand, sandstone and marl, and in some places the foot of it is made up of conglomerate and ammonite fossils (Paškevičius, 1997; Grigelis, 1994a). This formation occurs in the whole area of distribution of the Jurassic deposits and it marks the beginning of sea transgression (Paškevičius, 1997).

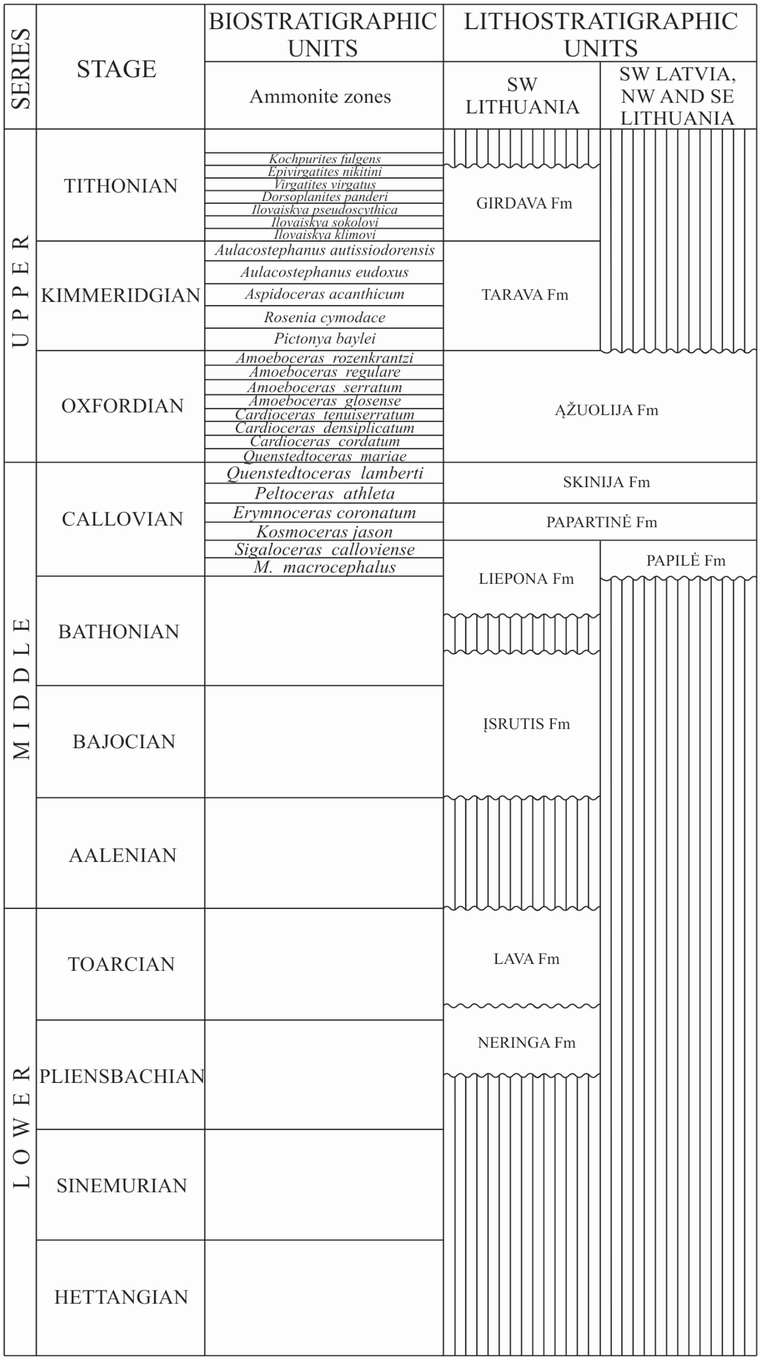

Figure 11. Stratigraphic chart of the Jurassic succession of Lithuania and Latvia (based on Paškevičius, 1997 for Lithuania; Stinkulis, 2004 and Paškevičius, 1997 for Latvia).

The Skinija Fm, up to 64 m thick, corresponds to the Upper Callovian (Grigelis, 1994b). In the northern areas of Lithuania, at the basin margin, it is represented by marl and sandy deposits with iron compound ooids (in the lower part) and micaceous clay and siltstone (in the upper part). South-westwards in the direction to the deeper part of the basin, the sandy deposits changes into black and grey micaceous clay and siltstone with pyrite and siderite inclusions and burrows (Paškevičius, 1997).

Middle and Upper Callovian deposits are also found in Latvia and well-characterised by ammonite, bivalve and foraminifera fossils. These deposits are composed of sandstone and clay, in places with carbonate concretions rich in sand grains and goethite ooids, as well as marine invertebrate fossils (Brangulis et al., 1998). However, due to the influence of Pleistocene glacial processes, these deposits are strongly deformed and even transported some distance (Strautnieks et al., 2006), and therefore their facies analysis and lithostratigraphic subdivision is problematic.

6.2.3. Upper Jurassic

The Upper Jurassic continues the succession of marine deposits. The Oxfordian Stage in Lithuania is represented by the Ąžuolija Fm, and three Oxfordian sub-stages are documented there. The Lower Oxfordian is composed of ooidal sandstone, clay, silt and siltstone, with a total thickness to 46 m (Paškevičius, 1997; Grigelis, 1994a). The Lower Oxfordian marks the maximum transgression of the Late Jurassic (Paškevičius, 1997). The Middle Oxfordian is composed of clay, silt, siltstone and sand. In southern Lithuania fossiliferous limestone with corals, silty marl and deposits rich in sponge spicules are documented. The thickness of the Middle Oxfordian in Lithuania is up to 6.5 m (Paškevičius, 1997). The Upper Oxfordian occurs in south-western Lithuania and is composed of ooidal sandstone, siltstone, carbonate-rich clay and limestone. Its thickness reaches 40 m (Grigelis, 1994a).

Oxfordian deposits, up to 1.6 m thick, have been documented in two boreholes in south-westernmost Latvia, near Rucava and Sikšņi. There the age of these silts and sands is determined based on finds of foraminfera (Gavrilova, 1979b). Recently an Oxfordian age has been also suggested for the Jurassic clays present in the glaciodislocated inclusion of the Jurassic clayey deposits within the Quaternary deposits at the Lose river mouth in south-western Latvia (Pipira et at., 2011). These palaeontological data indicate that in future studies it may be possible to trace the Callovian and Oxfordian formations documented in Lithuania and also in south-western Latvia.

The deposits of the Kimmeridgian Stage are distributed only in the south-westernmost part of Lithuania, but have never been documented in Latvia. The reduction of the distribution area is suggested to be related to basin retreat (Paškevičius, 1997). The Tarava Fm corresponds to this stage in Lithuania. The lower Kimmeridgian (lower part of the Tarava Fm) is represented by sandstone, silty argillite and clay, up to 54 m thick, but the upper Kimmeridgian (upper part of the Tarava Fm) by silty argillite, clay and glauconitic siltstone, up to 51 m thick (Paškevičius, 1997; Grigelis, 1994a).

The Tithonian Stage is distributed only in an isolated area in south-western Lithuania. The Girdava Fm is attributed to this stage (to the Lower and presumably also Middle Tithonian Substage) and is composed of carbonate-rich siltstone, silt, clay and marl. The total thickness of Tithonian deposits in Lithuania is up to 23 m (Paškevičius, 1997).

The distribution area of the Jurassic marine deposits gradually reduced from the times of the wide sea transgression in the Callovian to the Tithonian time (Šimkevičius, 2004).

6.3. Cretaceous

Cretaceous deposits are found in the Polish-Lithuanian Depression (Paškevičius, 1997). The maximum thickness of the Cretaceous succession in southern Lithuania is 200 m. From this area the deposits gradually thin out north-westward, but the thickness decreases sharply to north-east (Paškevičius, 1997).

6.3.1. Lower Cretaceous

There are no deposits corresponding to the Berriasian up to the Lower Albian in Lithuania (Fig. 12). The lower part of the Upper Albian is represented by the Užupis Fm composed of light-green non-carbonate cross-stratified sand with an admixture of glauconite, pyrite concretions and wood remains (Paškevičius, 1997). In the Šventoji River valley and the vicinity of Kaunas, the sandy deposits of this formation are coarse-grained, but south-westwards the sand grain-size decreases, cross-stratification disappears and the admixture of siltstone increases. The thickness of the Užupis Fm reaches 16 m (Grigelis, 1994b; Paškevičius, 1997). The deposits of the Užupis Fm are supposed to have been formed in deltaic settings with a dominance of fluvial processes (Paškevičius, 1997). The Užupis Fm is present only in south-eastern Lithuania (Radzevičius, 2004).

The 34-107 m thick Jiesia Formation, is present in all of the Cretaceous area of distribution. These deposits are composed of quartz and glauconite sand, siltstone and sandstone with phosphatic concretions (Grigelis, 1994b). In south-western areas, in the more offshore area of the Cretaceous basin, glauconite sand becomes finer, and the amount of clay and silt admixture increases (Paškevičius, 1997).

6.3.2. Upper Cretaceous

The Upper Cretaceous geological succession in Lithuania and the neighbouring Kaliningrad district (Russia) is complete and represented by the Cenomanian to Maastrichtian stages (Paškevičius, 1997).

The **Cenomanian Stage** is present in quite a wide area in southern Lithuania. The Lower Cenomanian Substage in the eastern part of southern Lithuania is represented by the Akmuo Fm, 2.5-5.4 m thick, composed of carbonate-rich glauconite sand and siltstone with phosphate inclusions. The Upper Cenomanian Substage in the same area is represented by the Kašėtai Fm, 1.6-4.9 m thick, made of glauconitic, sandy, clayey and chalky marl with phosphate concretions. In the western part of southern Lithuania, the Labguva Fm corresponds to the whole Cenomanian Stage. The lower part of it is composed either of glauconite conglomerate and a sandstone or phosphorite bed (Udra Member) dominated by phosphate concretions. The rest of the Labguva Fm is composed of quartz and glauconite sand, sandstone, sandy siltstone and clay with phosphatic concretions (Paškevičius, 1997).

The **Turonian Stage** is also widely distributed in southern Lithuania. In the eastern part of southern Lithuania the whole Cretaceous succession from the Turonian to the Maastrichtian is unified in the Voruta Group. Its lower part in this area is called the Pamerkys Fm and it corresponds to the Lower Turonian (Paškevičius, 1997; Radzevičius, 2004). The Pamerkys Fm is composed of white chalk and chalky marl with in-

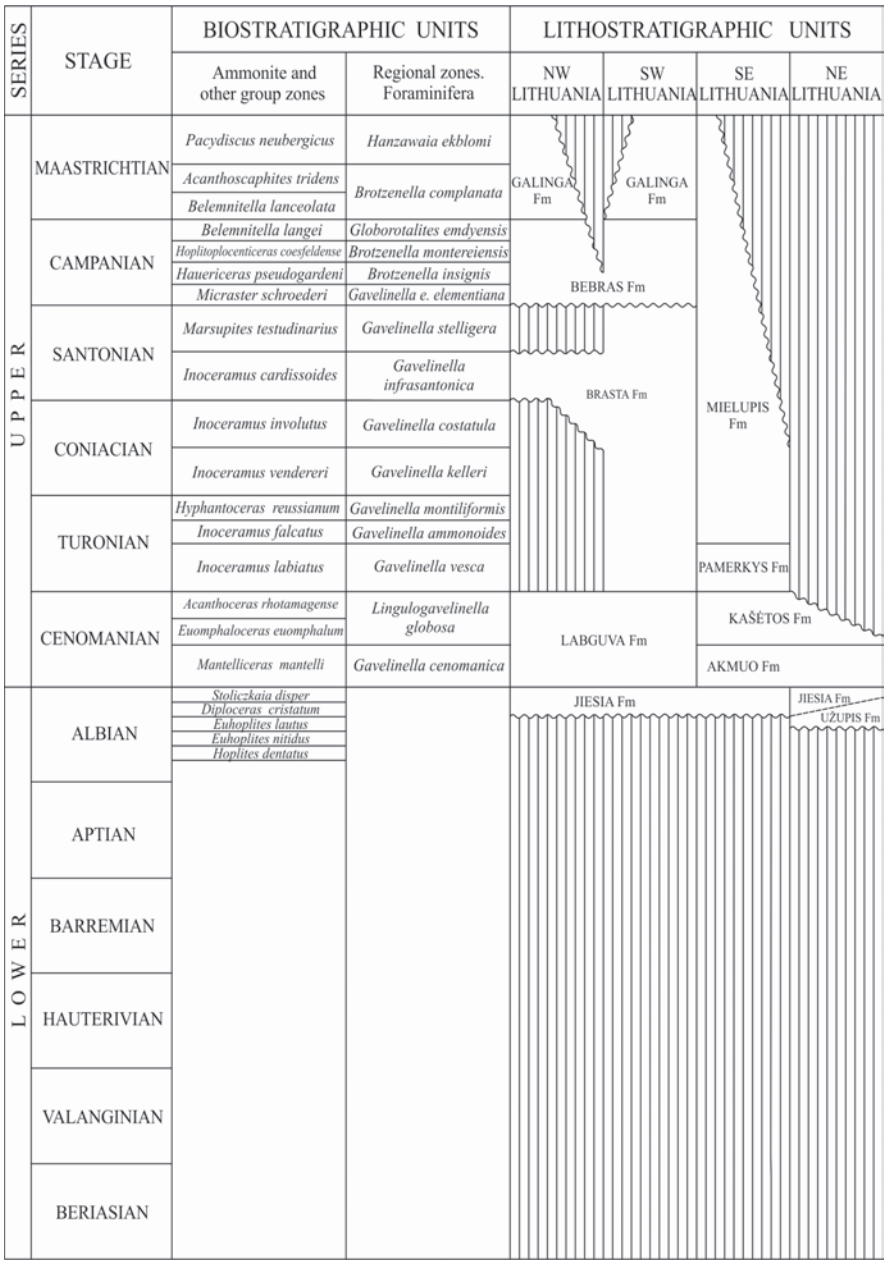

Figure 12. Stratigraphic chart of the Cretaceous succession of Lithuania (based on Paškevičius, 1997).

clusions of flint. Its thickness is 4-25 m (Grigelis, 1994b). In the western part of southern Lithuania the Brasta Fm is attributed to the Turonian to Lower Santonian. The Lower Turonian deposits in this area have been found only in the Vištytis-17 borehole. It is represented by sandy and chalky marl, as well as silt and silty sand (Paškevičius, 1997).

The Upper Turonian deposits in the eastern part of southern Lithuania are represented by chalk with flint, up to 27 m thick. These deposits and the rest of the Cretaceous succession, up to the Masatrichtian, in this area are unified in the Mielupis Fm. In the westernmost part of southern Lithuania the Upper Turonian is made of up to 43 m thick glauconite and carbonate-rich clay, sandy marl and chalk (Paškevičius, 1997).

The deposits of the **Coniacian Stage** are widely distributed in the eastern part of southern Lithuania, but are less well-represented in south-western areas. The Lower Coniacian Substage in eastern areas is made of chalk with flint. Deposits are sandier and also more silicified to the west. The Upper Coniacian Substage in the eastern areas is similar to the Lower one, but in the western part of southern Lithuania it is dominated by silty and sandy chalk and marl with glauconite and phosphate concretions. The total thickness of the Coniacian Stage is 42-65 m (Paškevičius, 1997).

The **Santonian Stage** is widely distributed in the eastern part of southern Lithuania but not so well-represented in western areas. In the eastern areas this stage is composed of chalk with flint, but in western areas contains more sand and is made of silicified chalk, opoka marl with glauconite, limestone and various siliciclastic deposits (Paškevičius, 1997; Grigelis, 1994b). The total thickness of this stage reaches 82 m (Paškevičius, 1997).

The **Campanian Stage** is present both in the eastern and western part of southern Lithuania (Paškevičius, 1997). In eastern areas this stage is represented by white chalk, which in an upwardly direction contains less sand admixture, but more opoka and flint inclusions. In western areas, the Bebras Fm is attributed to the whole volume of the Campanian (Radzevičius, 2004). The deposits of this formation are marls, chalky clay and siltstone, often silicified (Paškevičius, 1997).

The deposits of the **Maastrichtian Stage** are present in south-western Lithuania. Their distribution is influenced by later erosional processes. In these areas the Maastrichtian Stage is represented by the Galinga Fm, which is composed of silicified clay, siltstone and clayey sand. Eastwards, more chalk and chalky marl, as well as limestone appears (Paškevičius, 1997). The Maastrichtian deposits have a considerable thickness of up to 168 m (Grigelis, 1994b).

During the Cretaceous period, an open, generally warm water sea basin developed in the southern part of the south-east Baltics. Carbonate sedimentation with an admixture of clayey to sandy particles dominated there. Phosphate concretions are interpreted to be related to cold water current inflow in the sedimentary basin, but the intense accumulation of siliceous material with the wide development of sponges or other organisms with SiO_2 skeletons (Paškevičius, 1997). In southern Lithuania, this basin was deeper, but from the west there was an inflow of siliclastic material. Starting from the Turonian time the depth of the Cretaceous basin increased, probably to 200-500 m (Grigelis, 1994b).

7. Cenozoic succession

7.1. Paleogene

The Paleogene deposits are distributed in limited area in the south-westernmost Lithuania and also in southern and south-western part of Kaliningrad district (Russia). In south-westernmost Lithuania the Paleogene succession is represented by the Liubavas Fm (Lower Paleocene), Alkas Fm (Middle Eocene) and Prūsija Fm (Upper Eocene) (Paškevičius, 1997).

7.1.1. Lower Paleocene

The Lower Paleocene in south-westernmost Lithuania is represented by up to 56 m thick Liubavas Fm. Its basal part is composed of sand with quartz gravel grains, sandstone and sandy phosphatic deposits. Upwards follow fine-grained glauconite and quartz sand overlaid by similar quartz sand with carbonate-rich sand and sandy limestone interlayers. Besides, the Liubavas Fm contains lenses and interlayers of siliceous deposits (Paškevičius, 1997). The deposits of the Liubavas Fm likely formed in shallow basin of normal salinity (Katinas, 1994a).

7.1.2.Middle and Upper Eocene

The Lower Eocene deposits are not present in Lithuania. The Middle Eocene deposits are unified in the Alkas Fm. In south-westernmost Lithuania they are composed by quartz and glauconite sand with interlayers of marl, limestone and siliceous deposits. Thickness of the Alkas Fm in this area is up to 23 m (Paškevičius, 1997). The deposits of the Alkas Fm presumably are of relatively deep shelf origin (Katinas, 1994a).

The Upper Eocene is represented by the Prūsija Fm. In Lithuania the deposits of this unit are represented by up to 10,5 m thick silt and sand (Paškevičius, 1994). The sedimentary environment likely remained silimar to the Middle Eocene time (Katinas, 1994a). In the Kaliningrad district the Prūsija Fm is composed of various siliciclastics, including siltstone with abundant amber inclusions (Paškevičius, 1997).

Younger Paleocene deposits are not found only in the Kaliningrad district (Paškevičius, 1997).

7.2. Neogene

The Neogene deposits are found only in isolated patches in the southern and north-eastern Lithuania and also in westernmost part of Kaliningrad district (Russia). The **Miocene deposits** in Lithuania are represented by quartz sand with coaly siltstone intercalations (Paškevičius, 1997). The **Pliocene succession** is distributed wider than the Miocene sequence. These deposits are represented by fine-grained quartz sand with coaly clay and siltstone interlayers. The Anykščiai RS is present in north-eastern Lithuania, in the upper part of the Pliocene sequence. This regional stage is composed of rather poorly sorted cross-stratified quartz sand, sandy siltstone and silty clay with the total thickness up to 10 m (Paškevičius, 1997). The Neogene deposits are supposed to be of the terrestrial, fluvial to lacustrine, origin (Katinas, 2004). Their thickness reaches 45 m (Katinas, 1994b).

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Script based MOSYS system for the generation of a three dimensional geological structure and the calculation of groundwater flow: case study of the Baltic Artesian Basin

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Abstract

A fully script based MOSYS software package for generating a geological structure and for the modelling of groundwater flow has been developed. The script commands execute specific higher level geometrical, geological or computational tasks and allow for the achievement of repeatable modelling results easily, with minimum programming experience. The possibilities for the developed script system are demonstrated by creating the geological structure of the Baltic Artesian Basin (BAB), performing the calibration of the hydrogeological model and analysing the results.

Keywords: Baltic Artesian Basin; groundwater flow; numerical modeling; scripting

Introduction

The calculation of three-dimensional (3D) groundwater flow requires a model of a geological structure, which is mostly generated from several sparse data sets using sophisticated interpolation and extrapolation algorithms with many free alterable parameters. The programs used for the generation of geological structures (GoCAD, 2012) or the visualization of geological structures (Rockworks, 2010) include scripting possibilities in addition to the mainstream interactive manipulation of data. The script based execution of the hydrogeological model MODFLOW (McDonald and Harbaugh, 1989) is realized in mfLab (2010). The main advantages of script based systems are the compulsory documentation of all parameter settings and the resulting exactly repeatable geological structure.

The aim in the development of the MOSYS package is the creation of a fully script based package for the generation of a geometric model of a geological structure and the modelling of groundwater flow. The developed high level script commands are easy to use for scientists with minimal programming experience. The script is based on the Python programming language (Python, 2012).

The overall structure of the processing data for hydrogeological modelling is divided into 3 basic parts – the information base, the geometry model and the hydrogeological model, see Fig. 1. The information base is organized as a MySQL data base (MySQL, 2012) and a set of data files. The geometric model of the geological structure is built using this information. On the basis of the geometric model, the finite element mesh is built and the groundwater flow is calculated.

The execution of a certain version of script using a corresponding set of data files provides a unique result for the model (structure, mesh, hydraulic head), which can be exactly repeated using the same version of the script and data.

The theoretical background of the groundwater model used and the calibration procedure is described by Virbulis et al. (2012). This paper describes the MOSYS modelling system in more detail, especially the data sources and the high level script commands used for the creation of the geometric model. The goal of the detailed description is to provide the key concepts and principles of the model system, not to replace the user manual.

The possibilities of the developed MOSYS script system are demonstrated by creating the geological structure of the BAB, performing the calibration of the hydrogeological model and analysing the results.

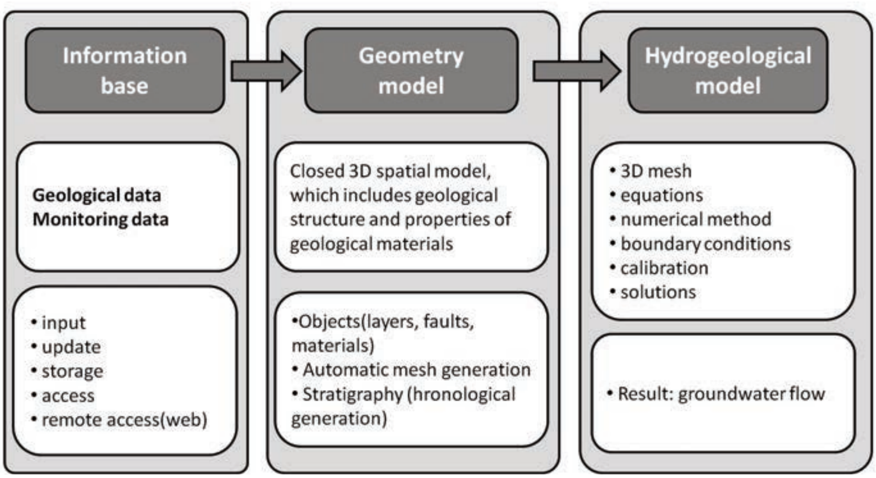

Figure 1. Schematics of the integrated model system.

Generation of the 3D geological structure and finite element mesh

Organization of data sources

The set of data files describes the definitive input data for the script. Various additional files are created during the execution of the script. These files are temporary and mostly used for debugging purposes, but they are also used for the data transfer between different modules and generation or calculation stages. Structure file and head file(s) are used for the analysis of the results.

The input data files have several types. These are shown in Fig. 2 and are described in detail in the next chapters.

Overview of the script

The script is written in the Python programming language (Python, 2012). The script commands, described later in detail, are Python subroutines executing specific higher level geometrical, geological or computational tasks. Some subroutines called windows executables, are written in the Delphi programming language. For example, the algorithms for building a/the 3D volume mesh from data sources, shown in Fig. 2, can be realised using the subroutines.

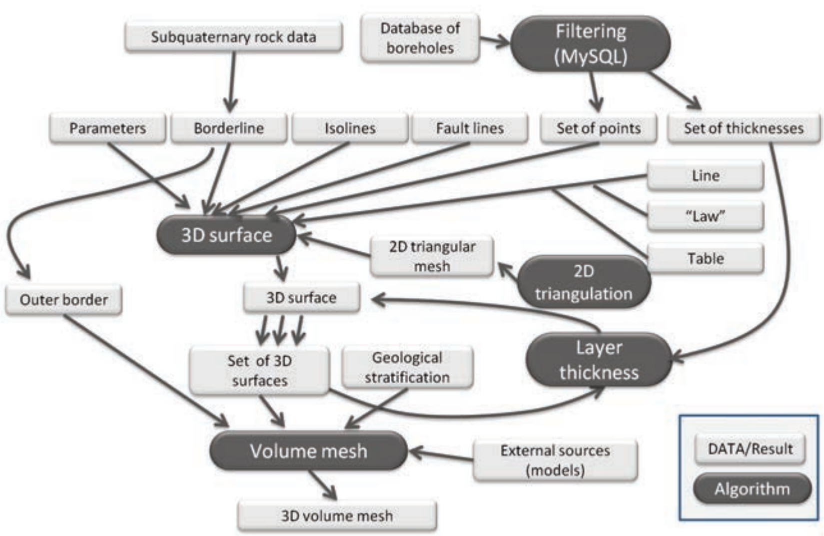

Figure 2. Overview of the algorithm for the generation of a geological structure.

Lines

The creation of line networks is the first step in the building of the geological structure i.e. the 2D mesh. There are several types of lines (generally open or closed polylines) which are necessary in the model or which increase the precision of the geometry ensuring the coincidence of geometric features and mesh elements. The boundary line of the domain prescribes the location of the side boundaries. The coastlines typically divide different kinds of surface boundary conditions (fixed pressure on the seabed and the infiltration rate on land). The boundary conditions with fixed pressure can be prescribed on rivers and the use of river lines enhances the representation of the earth's topography. The borders of the distribution of geological layers (mainly taken from geological maps) ensure that layer boundaries coincide with the edges of mesh elements. The borders of countries or administrative districts are included in order to be able to prioritize information sources in different areas. Fault lines are also included in the model in order to shift the elements of the 3D mesh vertically along the faults. Any other lines necessary for the model (e.g. lakes) or improving the quality of the mesh (isolines of earth surface, areas for mesh refinement) can be added to the mentioned types of lines.

Sets of lines can be loaded from GIS shp files, from a MODFLOW mesh file as boundaries of the mesh (if information of the MODFLOW mesh is included as a part of the model) and from a simple text file easily created in text editor or inside the python script.

The line network is created by the subsequent adding of lines to the network structure. The structure includes information about points (number, identificator, coordinates) and polylines (number, identificator and list of points), so there are no double points in the line structure. To ensure this clean structure, several algorithms are used during the adding of line sources to the structure:

1. add set of lines (Merge);
2. remove closed areas smaller than specified area (RemoveSmallAreas);
3. merge points closer than specified distance (MergePoints);
4. project points on near lines closer than specified distance (MergeCommonEdges);
5. intersect lines inserting point (Intersections);
6. remove segments going back and forth along the same line (RemoveTrivialPoints);
7. change the direction of polygons if necessary (NormalizePolygons);
8. delete unnecessary points on straight parts of polylines (SimplifySingleLines);
9. remove double edges (RemoveDoubleEdges);
10. remove free standing points without lines (RemoveSinglePoints);
11. eliminate small angles between lines (RemoveSmallAngles).

Some operations are repeated iteratively after adding the next set of polylines until these operations have no more effect on the structure. The resulting structure consists of lines and polygons with a certain generalization level which can be accessed by an identifier in later stages of the building of the model. Sets of lines can be loaded using the function Load and saved using the function Save.

2D mesh

2D triangular mesh is built based on the network of lines. Additionally, points can be added as mesh nodes e.g. the locations of boreholes where the stratification is well known or which will be later used for calibration of the hydrogeological model.

The utility Triangle is used for 2D Delauny triangulation (Shewchuk, 2002). Edges of generated triangles cannot cross the segments of the line network, but segments can be split if necessary. The target area of triangles should be specified and can be different in each polygon. As some lines can cross the border of the computational domain, the mesh is generated in a larger area and only later elements lying inside the boundary line of the domain are kept in the mesh.

The next operation is the inclusion of faults into the mesh by cutting the mesh along all fault lines i.e. duplicating the points on these lines. The result is a basic or global 2D mesh which is used as a basis for the building of other compatible meshes e.g. where the deep faults are joined in upper layers or temporary meshes for specific operations in smaller areas (function CombineCuts). The point and triangle numbering is global and the data can be shifted between all compatible meshes. The mesh file is called meb-file further in the text.

Surfaces

The building of surfaces of geological layers is the most complicated step during the creation of a/the 3D geometric structure. The main data object, used during the generation of surfaces, is the file containing a sub-set of points with information about the point number in the global mesh and the value (mostly used for z-coordinate) in each point, called z-file. Z-files are often used also for selection of certain areas or lines. Another important data file contains a subset of elements (triangles) containing the global triangle number and one value in each triangle, called ez-file. Additionally, files containing sets of x-,y- and z-coordinates of points (called xyz-files) not related to the numbering of the mesh points are also used.

Table 1. The list of basic level functions often used in surface generation.

Function	**Purpose**
ZFileOp	performs logical and arithmetical operations with z-files
SelectMeshRegion	selects region of mesh inside or outside of polygon (defined in line network) and writes it to meb-file
StringToFile	writes the string in file
MergeZFiles	equivalent to ZFileOp with logical operation OR
Merge	Merges content of two files
SQLToTXT	writes the result of SQL data base query to the text file
XYZToZ	interpolates the values from points to the vertices of 2D mesh
ImportFromSHPToOneGroup	imports the lines from shp-files into line data base
SubMeshByZFile	selects region of mesh and writes in meb-file
ExtrapolateZ	sets the average value of points inside of defined distance around the points where values are not defined
KernelExtrapolationMACRO	Performs subsequent execution of KernelInterpolate
SHPToZ	joined functions SHPToXYZ and XYZToZ
MeshToXYZ	Transfers mesh point coordinates from meb-file to xyz-file
ReadXYZFile	Reads content of xyz-file into memory

LuzLineSHPToLuzDB	Transfers height information on both sides of fault from shp-files to fault data base
ImportFromMeshBorder	Puts border line of mesh to line database
FromDBToTXT	Writes height or thickness information of selected geological layer to text file
InterpolateLuzumi	Transfers the information from fault data base to z-file
KernelInterpolate	Calculates the value from weighted values in neighbour points.
LuzSHPToLuzInfo	Imports fault lines and height information
Smooth	smoothes the values in mesh points
XYZFileOp	Performs logical operations with XYZ files
LuzInfoToXYZ	Transforms fault database to xyz-file
CombineCuts	"glue" cuts in 2D mesh – joins double points together in one point
InterpolateFromRaster	Interpolates information from GeoTIFF-file to meb-file mesh points
SHPToXYZ	converts the coordinates and specified field in points from shp-file to xyz-file format
ImportFromSHP	Imports lines from shp-file to line database
ImportFromSHPByFields	Imports the lines from shp-files into line data base
getSQLHeadInLayer	Writes observed heads from selected layer to xyz-file
getSQLHeadInLayerCor	Writes density-corrected observed heads from selected layer to xyz-file
SaveOptHistory	Saves the target functions and material properties during the optimization procedure in text file
GetSQRDeviation	Calculates target function from str-file, p-file and set of observed heads
AlphaShape	Smoothes border line, created from set of points
MakeMeshFromXYZ	Triangulates set of points
WriteZFile	Writes values to z-file
WriteXYZFile	Writes variables to xyz-file

A set of functions, manipulating and transforming data in meb-, z-, ez- and xyz-files, is defined and used in the script. There are lower level functions executing some basic level actions and higher level user defined functions generating the whole surface. The list of basic level functions often used in surface generation with short explanations is given in Table 1. Some of the most important and often used functions will be explained closer here.

The function SQLToTXT returns the result of the SQL data base query to the text file and is often used to create an xyz-file containing the values of layer positions in boreholes. Function StringToFile writes the string in file and is mainly used to create simple xyz-files directly inside the script instead of adding them to the set of input data files.

The function SHPToXYZ converts the coordinates and specified field points from shp-file to xyz-file format. Functions ImportFromSHPToOneGroup and ImportFromSHPByFields import the lines from shp-files into line data base. Function

XYZToZ interpolates the values from points, contained in the xyz-file, to the vertices of the 2D mesh of the specified meb-file and the result is written in a compatible z-file. During this operation a temporary 2D mesh is built using only the points from the xyz-file and the values are linearly interpolated to the points of the target mesh. Both functions SHPToXYZ and XYZToZ are joined in one often used function SHPToZ.

The function ZFileOp performs logical and arithmetical operations with z-files. The logical operations are AND (intersection), OR (union), DIFF (complements) and SDIFF (difference) and these prescribe the resulting set of points. Arithmetical operations are performed point-wise and any formula in python syntax containing values in two input files is allowed. The often used function MergeZFiles is equivalent to ZFileOp with logical operation OR. The function SelectMeshRegion selects a region of mesh inside or outside of a polygon (defined in line network) and writes it to the meb-file. Another method of selecting a region of mesh is using the points in Z-file (SubMeshByZFile).

The function ExtrapolateZ sets the average value of points inside a defined distance around the points where values are not defined. Another extrapolation function is KernelInterpolate. This function calculates the value from points inside a defined distance and the weight of each point is exponentially decreased with the distance between points. Function Smooth smoothes the values in mesh points.

Direct definition of values in a whole sub-mesh is invoked using functions MeshSetValue in points for z-files and MeshSetElValue in ez-files. Constant values or functions can be set.

Special algorithms are introduced for the incorporation of structural faults into the mesh. Fault lines, added to the line set for 2D mesh generation, also have height information on both sides of the fault, transferred from shp-files to a special data base using the function LuzLineSHPToLuzDB. This data base information is transferred to z-file using the function InterpolateLuzumi. Later this z-file together with height information from other sources is used for the construction of geological surfaces.

The above described functions (and also others that are not described, but are not principal) are used for the generation of geological surfaces. As an example, the generation of the crystalline basement surface in the model of the BAB (v0) is described here. From the isolines of the basement map of the BAB the z-file is created (function SHPToZ). The height information of faults in the basement map is saved to fault data base (LuzSHPToLuzInfo) and written to an xyz-file. The height information from available boreholes in Latvia is also saved to an xyz-file. Then the obtained z-files are merged with information about the basement height on the border of the BAB and the height information at two points in Belarus. From the resulting xyz file the z file is created using linear interpolation (function XYZToZ). After that the height information along faults is interpolated from fault information to all mesh points along faults and both z-files are joined (MergeZFiles) and smoothed (Smooth). These values are transferred to the sub-mesh of Latvia. In the territory of Estonia the basement surface is interpolated from an available raster file (InterpolateFromRaster) and in Lithuania from a shp-file. Now all four z-files (the whole BAB, Estonia, Lithuania, Latvia) are joined where the BAB has the lowest and Latvia the highest priority.

During the construction of higher positioned surfaces other algorithms are used, too. One of them is the use of layer thickness to construct the surface above (because the thickness information has less error sources than the absolute height). The thin aquitards are also specified by one constant thickness. Another principal algorithm used is the inclusion of known erosion surfaces as a sub-quaternary surface. If some layer lies directly under the Quaternary layer, the surface of this area is aligned with the erosion surface, which is usually smoother and better known.

The surfaces are generated starting from the deepest surface. If some layer is not present in the whole domain but only in some smaller area, the layer thickness is defined as in the left area – i.e. the upper surface is set in the same position as the previous deeper surface.

3D structure

The script system allows one to easily define complex structures as a quaternary sequence with varying material properties inside one layer or spatially vanishing layers.

The 3D structure is constructed from the set of surfaces defined above. Additionally, material properties must be defined for each layer between two surfaces. The material properties must be set in all elements of each layer using an ez-file. The value is assumed to be constant within each element. The procedure GenerateStructure requires a 2D mesh as input, a list of surfaces (layers), a list of ez-files with material properties for each layer, and a list of colours for each layer. The output of this procedure is a structure file *.str. The generated structure consists of triangle prisms, pyramids and tetrahedrons. At the same time the structure is also the 3D element mesh, used for the calculation of groundwater flow.

Hydrogeological model

Calculation of groundwater flow

A 3D Darcy flow with free-surface and anisotropic conductivity is assumed for the steady-state solution:

$$\frac{\partial}{\partial x}\left(K_{xy}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{xy}\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_{z}\frac{\partial h}{\partial z}\right)+q=0 \quad (1),$$

where h is the piezometric head, q are the sources of water abstraction and K_{xy} and K_z are the horizontal and vertical hydraulic conductivities. The possibility of calculation of groundwater flow and piezometric head is also included in the MOSYS script, and the function Calculate solves the steady state equation. This function requires the 3D structure str-file, the initial conditions and boundary conditions as input.

Boundary conditions are limited to two kinds. The value of the piezometric head (in points) or flux (in elements) must be set at the upper boundary. The side and bottom boundaries are defined as impermeable in the present version of the function Calculate. The water extraction must be also prescribed, if present. This is done by providing coordinates x,y,z and the extraction value. This is a reasonable simplification as only one element is present per layer thickness.

Function CalculateUnsteady is used for the simulation of unsteady groundwater flow

$$S_S \frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left(K_h \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_h \frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_v \frac{\partial h}{\partial z}\right) + Q(t) \quad (2),$$

where S_S is storativity and *q(t)* are time dependent sources of water abstraction. Additionally, this function requires the distribution of water abstraction in time, starting time, end time and the time step for the simulation run.

The results – piezometric heads in every mesh point - are written in *.p file containing one field in a steady state case or series of heads in an unsteady case.

Calibration of the model

The calibration of the hydrogeological model is one of the most important steps during model development. The possibility of calibration i.e. the optimization of material properties (filtration coefficients) is included in the script as well. The optimization method L-BFGS-B is used for the calibration of the model. This is a quasi-Newton optimization method where the storage for the Hessian matrices is limited according to Nocedal (1980). The procedure *fmin_l_bfgs_b* implemented in the Python optimization library "s*cipy.optimize*" by Scipy (2011) is used for the calculations.

First the history file can be cleaned (function ClearOptHystory) and then the optimization run can be started (function OptimizeParams). First the parameters to optimize are defined (e.g. filtration coefficients for each layer and one coefficient for infiltration) together with the initial values and the range of parameter change (0.01 – 100 from initial values). The function for the calculation of the optimization target compares the observed values of the piezometric heads in selected points with the calculated ones. The optimization procedure chooses new parameter values depending on the target function. During each optimization iteration, the material properties are changed, the structure with new material properties is generated and the calculation of piezometric heads is carried out.

Post-processing

Several post-processing possibilities are included in the script. Function GetResultsAt prints the values of piezometric heads in locations x,y,z specified in an xyz-file. This function is also used during the optimization procedure to get the calculated heads in boreholes where the observations are available. Function MeshToVTU converts the mesh to vtu format, which can be analyzed using the software ParaView (Paraview, 2012). Function MebToJpeg plots the iso-surface of a field specified in a z-file on a given 2D mesh (meb-file). Function WaterBudget integrates the water flow between layers in a selected area and prints the sums of positive, negative and total water fluxes in text file.

Additional analysis can be carried out using interactive post-processing tools. MOSYS output data format is compatible with HiFiGeo (HiFiGeo reference). HiFiGeo allows one to perform analysis of calculated and observed heads and flow fields in horizontal and vertical sections, polylines, surfaces of geological layers in 3D views as well.

The data can be converted to ParaView vtk format using the utility StrToVTK.

This utility allows one to export a selected layer or all layers from a str-file. The piezometric head, conductivities, mesh related variables (volume and area of finite element) and variables calculated by StrToVTK, such as pressure and artesian pressure can be exported as well. ParaView is an open-source, multi-platform application designed to visualize data sets of varying sizes (Paraview, 2012). It includes the possibility of Python scripting for automatization of analysis.

Case study - Baltic Artesian Basin

The possibilities of the developed MOSYS script system are demonstrated on the basis of the BAB. Several geometries are generated and calculations of groundwater flow carried out for the BAB using MOSYS. Calculations based on the geometry version V0 consisting of 24 layers are published by Sennikovs et al. (2011). The geometry version V1 with 42 layers is presented first by Sennikovs et al. (2012). The calibration of V1 is presented by Virbulis et al. (2012b) and the results by Virbulis et al. (2012c).

Geological structure

There are many sources of data on the geological structure of the BAB. The heterogeneous information from different sources, which are employed for the building of the geometrical structure of the model, are unified. The information sources include:

(1) Structural maps of the topography of several formations for Latvia (4 maps) and Lithuania (13 maps, the database of the State geological survey of Lithuania), Brangulis et al. (1998);

(2) Geological maps of the sub-Quaternary for Latvia and Lithuania;

(3) Structural maps of the crystalline basement in Latvia and BAB, Brangulis et al. (1998) and Vetrennikovs (1996);

(4) Data for around 20,000 boreholes in the territory of Latvia from the database of the Latvian Environment, Geology and Meteorology Agency (LEGMA);

(5) Geological model of Estonia by Vallner (2003);

(6) Surface topography from SRTM data with 25 m resolution, Jarvis et al. (2008);

(7) Bathymetry of the Baltic Sea by Seifert (2001);

(8) Data from published geological cross-sections;

(9) Literature studies: Vetrennikovs (1996), Sorokin et al. (1981), Kovalevskij (1967), Brangulis (1985), Ulste (1961), Tuulig and Floden (2009).

The triangular mesh in the horizontal plane is constructed so that it incorporates characteristic lines such as rivers, coastlines, borders of countries and areas of the distribution of geological layers. The boreholes later used for calibration are also included in the mesh as nodes. Additionally, fault lines are also taken into account – the 2D mesh is cut along the fault lines and the mesh points are duplicated along them. The target area of triangles is non-uniform, starting from 10 km^2 in areas with dense geological information (Baltic States) up to 100 km^2 in the area of the Baltic Sea. The side length of the triangles is even smaller near the lines and points included in the mesh. The top view of the surface mesh is shown in Fig. 3.

The geological structure consists of 42 layers distinguished on the basis of each geological unit's hydraulic properties and geological data resolution. The number of layers is allowed to vary across the domain. It includes aquifers and aquitards from Vendian up to the Quaternary deposits. The Quaternary layer is divided into 4 layers according to Jatnieks et al. (2012). The cross section along the line AB in Fig. 4 illus-

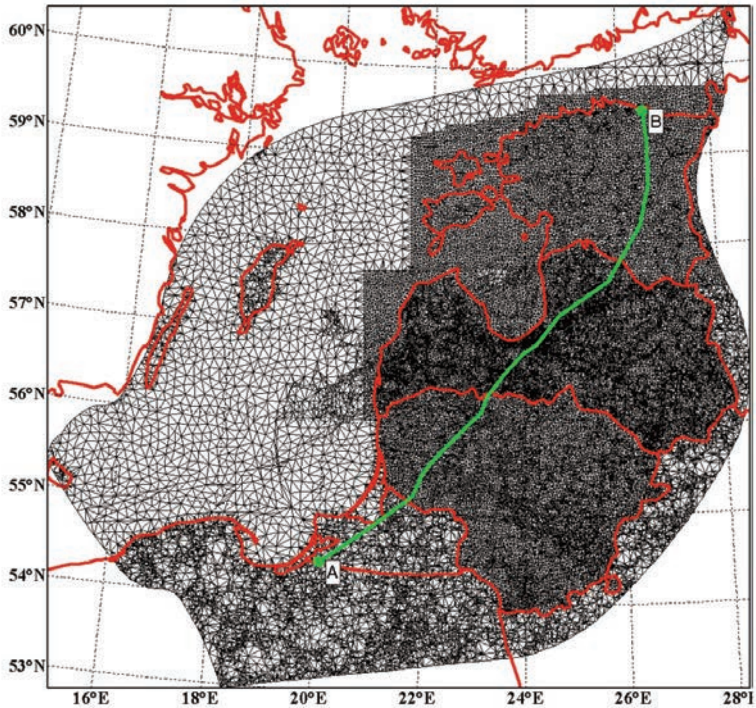

Figure 3. Triangular 2D base mesh of the BAB. Red lines – borders of the countries. Green line – cross-section AB.

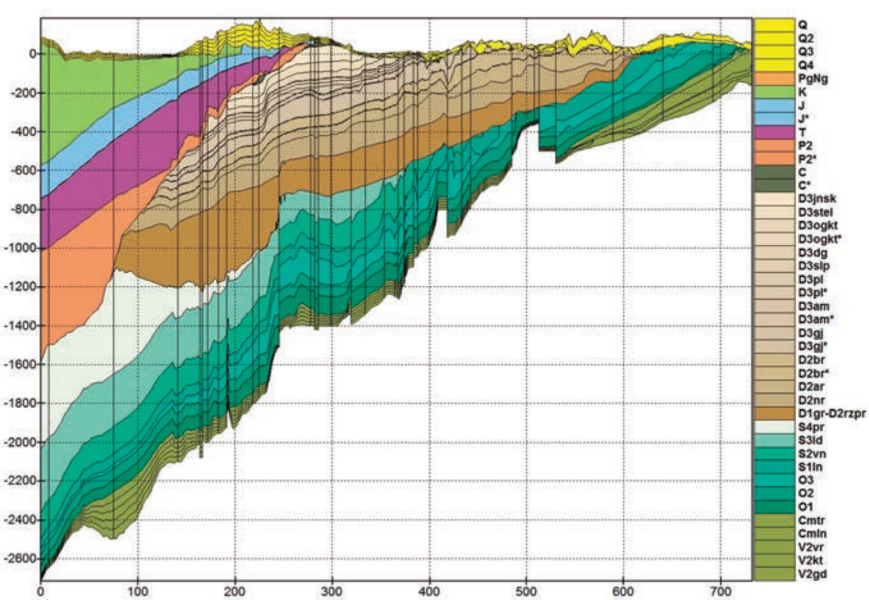

Figure 4. The cross-section of the BAB along the line AB (see Fig. 3 for the cross-section line position).

trates the geological structure of the BAB. The symbol * was used for those aquitards which have the same name stratigraphical unit as an aquifer.

The/A Quaternary sequence is treated as a four layer structure with a variable number of layers across the domain. Fault displacements are incorporated into the model taking into account data from the published structural maps. Four reconstructed regional erosion surfaces (upper Ordovician, Devonian, Permian and Quaternary) are considered during the building of the model.

Hydrogeological model

Boundary conditions

The Precambrian basement forms the impermeable bottom of the model as suggested by Levins et al. (1998) and Mokrik (1997). On the northern and western side of the BAB the basement reaches the earth's surface and the thickness of the model is zero. On the south-western side, the BAB borders the Danish-Polish basin with a zone of extensive faulting and this boundary is assumed to be impermeable according to Mokrik (1997). The eastern side of the BAB is connected with the Moscow Artesian basin and the south-eastern boundary is the Belarus-Masurian anticline. The thickness of the BAB at these boundaries is approximately 300 – 500 m. Zero water exchange is assumed through these boundaries.

A simple hydrological model is applied on the surface. The level of the lakes, rivers and the sea is fixed as a constant hydraulic head in corresponding mesh points. The infiltration is set as a flux boundary condition in surface elements which contain at least one point where the hydraulic head is not fixed. The results of the regional climate model KNMI-RACMO2 with 25 km resolution from the ENSEMBLES project are used for the spatially distributed infiltration field calculation (ENSEMBLES, 2008). The infiltration field is constructed as a weighted difference of 30 year averaged precipitation and evaporation fields. The weight value is calibrated during the optimization procedure.

Groundwater abstraction data in Latvia, Lithuania and Estonia is used to set-up the sources of water abstraction. Only abstraction wells with large yields are taken into account. A total of 49 wells in Lithuania (total abstraction 45,000 m^3/day), 161 in Latvia (184,000 m^3/day) and 172 in Estonia (24,000 m^3/day) are considered. Each q [m3/s] source was distributed inside the enclosed finite volume element.

Model calibration

The model is calibrated on the available head measurements in monitoring wells and head measurements in boreholes during the installation. The data is available from the year 1913 until the present, however, 90% of the boreholes were installed after 1962 (99% after 1953). 90% of the monitoring well data is measured after 1972. As the available data is not uniformly distributed over the covered area, a spatial weighting coefficient was assigned to each borehole to avoid overestimation of the borehole clusters (Virbulis et al., 2012).

The monitoring data shows distinct time dependence of the water level in aquifers intensively used for groundwater abstraction. As the model is steady-state, the year 2000 is chosen as the reference year for the present time scenario. The data taken specifically in this year is insufficient, therefore, observations from surrounding years are also taken into account but with smaller weighting coefficients (Virbulis et al., 2012).

The target function Z_j of layer j is the weighted sum of squared differences between observed and modelled piezometric heads (Virbulis et al. 2012). The overall target function Z, which is minimized by the optimization method L-BFGS-B, is the sum of Z_j. The equal importance of each layer is assumed and no coefficients are used in this sum.

The water in the deep layers of Cm and O-S has high salinity and, respectively, density up to 1.08 g/cm^3 according to Levins et al. (1998). Therefore, the observed heads in the Cm aquifer are corrected to virtual fresh water heads by multiplying the water column between the top of the O-S layer and the water level in the borehole by the density ratio measured in the corresponding borehole.

The parameters of the calibration are the horizontal and vertical hydraulic conductivities of the hydrogeological layers. The initial values of the conductivities are taken from the available field pumping test measurements or based on the lithology of individual hydrogeological layers. The vertical conductivities are decreased 10 times in aquifers considering the anisotropic structure of the sedimentary layers. One coefficient per layer (S-O layers are grouped and have one coefficient) is changed during the optimization, i.e. the ratio between the horizontal and vertical conductivity is kept fixed in each optimization run. There are 37 calibration parameters altogether - one for each of the 36 layers (layer groups) and one for the multiplication of distribution of infiltration.

The minimization of objective function typically converges in several hundreds of iterations, see Fig. 5. Each iteration takes about 5 minutes on i7 PC with 8 cores, direct solver is used, and the mesh consists of about 3 Mio elements.

Table 2. Initial and optimized values of hydraulic conductivities [m/day] for case 1 and case 2.

layer	Initial	case 1	case 2
Q	10.0	13.8	6.4
Q2	0.0001	0.0010	0.0022
Q3	10.0	3.0	1.2
Q4	0.0001	0.0010	0.0023
PgNg	10.0	16.3	8.3
K	2.0	2.1	2.2
J	1.0E-06	2.7E-07	2.7E-07
J*	10.0	100.0	104.9
T	1.0E-06	1.0E-05	4.7E-06
P2	1.0E-06	1.2E-07	2.1E-07
P2*	2.0	0.9	0.7
C	2.0	3.4	5.3
C*	1.0E-04	3.8E-04	7.9E-04
D3jnsk	2.0	0.3	0.3
D3stel	1.0E-04	3.4E-05	7.3E-05

D3ogkt	2.0	0.6	1.2
D3ogkt*	1.0E-05	1.7E-06	2.3E-06
D3dg	10.0	1.8	0.8
D3slp	1.0	0.2	0.5
D3pl	10.0	2.7	1.3
D3pl*	1.0E-07	1.3E-08	2.5E-08
D3am	2.0	0.5	1.1
D3am*	1.0E-07	2.7E-07	5.3E-07
D3gj	2.0	2.4	5.2
D3gj*	1.0E-07	1.0E-06	1.0E-06
D2br	2.0	0.3	0.7
D2br*	1.0E-07	3.3E-07	6.5E-07
D2ar	2.0	0.5	1.0
D2nr	1.0E-09	1.8E-09	7.7E-10
D1gr-D2rzpr	2.0	0.7	0.7
S4pr	0.010	0.008	0.019
S3ld	10.0	8.4	18.8
S2vn	0.010	0.008	0.019
S1ln	10.0	8.4	18.8
O3	0.10	0.08	0.19
O2	10.0	8.4	18.8
O1	1.0E-05	8.4E-06	1.9E-05
Cmtr	1.0	0.6	0.2
Cmln	1.0	1.0	2.1
V2vr	1.0	0.5	0.2
V2kt	1.0	1.0	1.7
V2gd	1.0	2.5	5.2

The initial values of the hydraulic conductivities for both cases are shown in Table 2. Case 1 (blue line) is started using initial parameters from optimization runs in previous studies and manual calibration. Case 2 (red line) is started using the optimized values from case 1 (also shown in table 2). Further reduction of the target function takes place while some conductivities reached the bounds of allowed change during the first optimization run (table 2). The development of some conductivities during the calibration procedure is shown by Virbulis et al., 2012b).

Dividing the overall target function Z by the number of layers N used in building the target function and taking the square root gives the average root mean square error (RMSE) values of 7.4 m (case 1) and 6.8 m (case 2). The values of BIAS (mean difference between observed and calculated head) and RMSE measures for each layer used for the estimation of model calibration quality are shown in Table 3. It can be seen that BIAS is smaller than +/-5 m for all layers in case 2. The RMSE values in the deeper layers Cm and D 1-2 are larger than 10 m but less than 10 m in all other layers, the corresponding relative RMSE value being less than 5%.

The correlation between the observed heads (years 1995-2005) and the modelled head (year 2000) for case 2 (red line in Fig. 5) is shown in Fig. 6. The correlation with

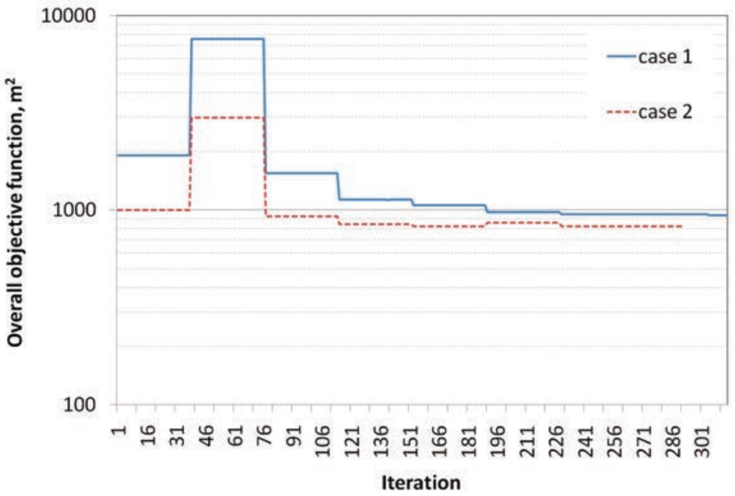

Figure 5. Development of objective function during the optimization for case 1 (blue line) and case 2(red line).

Table 3. BIAS [m] and RMSE [m] for layers used in the calculation of the target function for case 1 and case 2.

Layer	Case 1		Case 2	
	BIAS, m	RMSE, m	BIAS, m	RMSE, m
Cm	1.3	15.0	4.2	11.7
D1gr-D2rzpr	5.2	9.7	-1.2	10.3
D2nr	0.0	7.6	1.8	7.0
D2ar	-0.8	4.9	-0.4	3.2
D2br	-1.3	4.9	-1.7	4.5
D3gj	1.9	10.0	1.0	9.8
D3am	-0.4	6.6	-0.5	6.8
D3pl	-2.4	6.1	-1.4	6.1
D3slp	-2.2	3.6	-1.9	3.8
D3dg	-2.6	8.9	-3.3	9.1
D3ogkt	-2.6	6.6	-1.9	6.5
D3stel	-3.5	4.5	-2.5	3.9
D3jnsk	-1.9	6.2	-1.8	5.8
C1	1.0	8.1	-0.3	6.3
P	3.3	8.1	3.4	6.7
T	-2.7	3.3	-3.4	4.1
J	3.4	3.4	4.4	4.4
Q	-1.3	5.5	-0.3	5.3

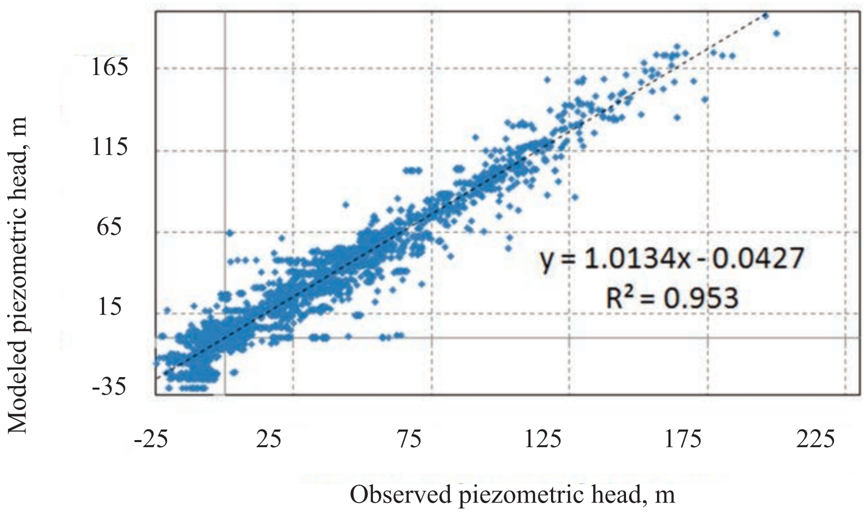

Figure 6. Modelled heads as a function of observed heads.

R^2=0.953 is very good and comparable with relative RMSE values. This result can be considered as validation because the calibration is done using time and spatial weights, but in this graph the observations between 1995 and 2005 are plotted and they have equal weights for the building of the linear regression line and corresponding R^2 measure. It can be seen that for most of the outlayers the modelled piezometric head value is less than observed. Most of them are located in places where the water abstraction is concentrated in one well when in reality it may be distributed over the administrative district.

Analysis of the results

Results yielded by calibration case 2 with the smallest target function are used for further analysis. Considering the large area of the BAB the results show general flow structures and cannot describe any local phenomena. The structure of the groundwater flows in the BAB will be analyzed along the layer surfaces as well as in the vertical cross-sections.

Fig. 7 shows the distribution of vertical velocity of water flow on the top of the Quaternary layer. Negative velocities represent recharge and positive velocities – discharge. The recharge takes place mainly at high elevations on land, intensive discharge at low elevations on land (lowlands, valleys of rivers) and slow discharge at the ground of the Baltic Sea. This distribution is the result of combined fixed head and constant infiltration boundary conditions.

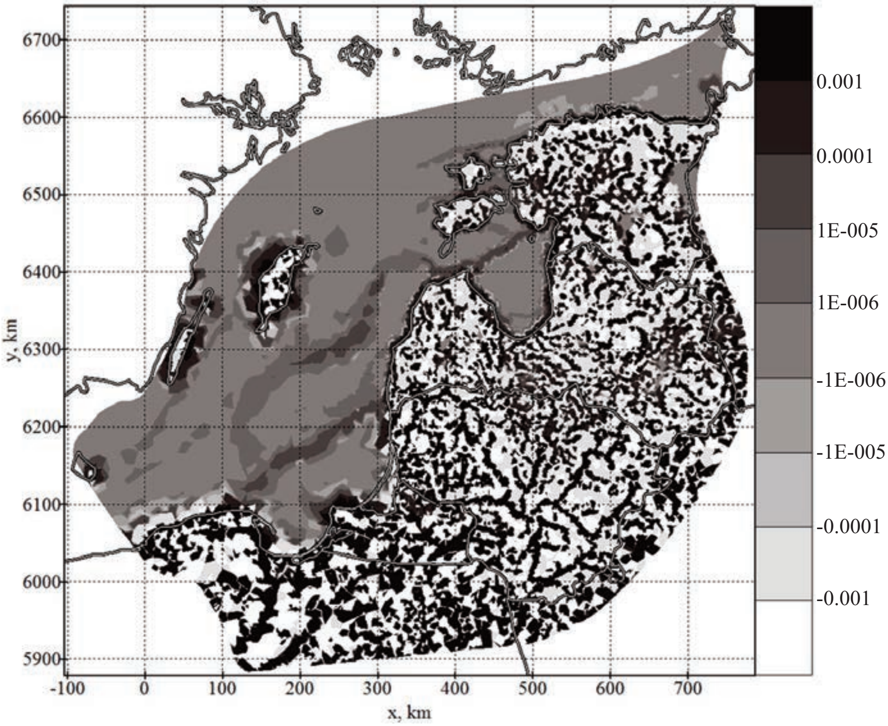

Figure 7. Vertical velocity [m/day] at the top of the Quaternary layer in logarithmic scale. Negative values represent recharge and positive values – discharge.

Equipotentional lines of the piezometric head are shown in two layers – the Cambrian Tebra (Cmtr, Fig. 8) and the upper Devonian Gauja (D3gj, Fig. 9). In the Cmtr layer, which represents the groundwater flow in deep aquifers, the recharge area is located in the south-eastern part of the BAB, where the Cmtr reaches the earth's surface coinciding with the highest elevations in the surface topography. In the northwest side of the BAB where the crystalline basement reaches the surface (coast of Sweden and Finland) the Cmtr layer has a discharge area due to a lower surface elevation compared to the SE side.

In the D3gj layer (Fig. 9), which is a constituent of the upper active exchange zone according to Levins et al. (1998), the general flow structure is similar – recharge in the higher eastern part and discharge in the lower western part. However, in this layer more local features are present as a discharge area in the Gulf of Riga where water flows from both the East and the West. High local gradients are present in the northern and south-eastern parts of the D3gj layer, where it reaches the sub-Quaternary surface. Discharge is also present in the valleys of the rivers Gauja (north) and Daugava (east) where the D3gj reaches the earth's surface.

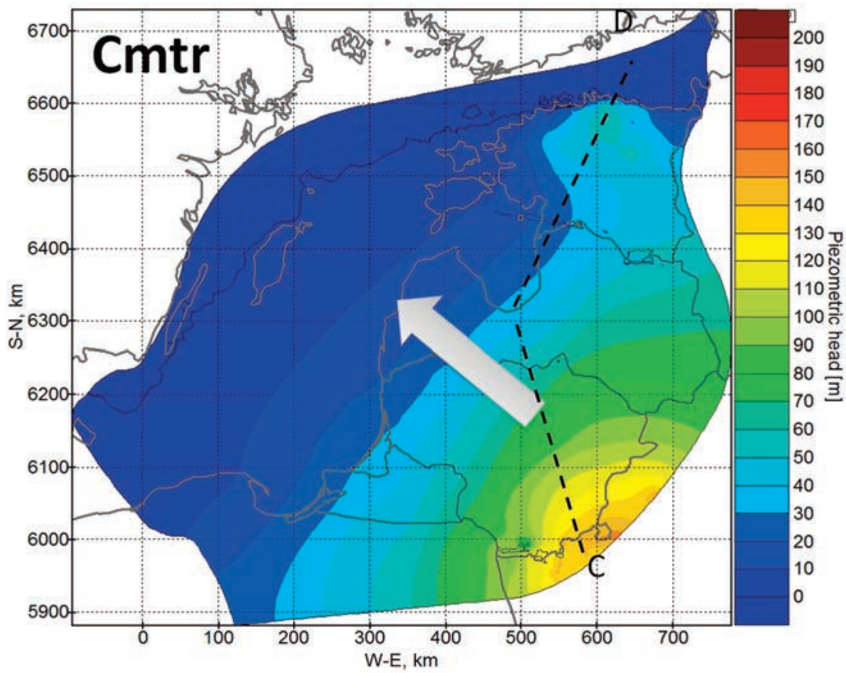

Figure 8. Piezometric head distribution in Cambrian Tebra formation (Cmtr layer).

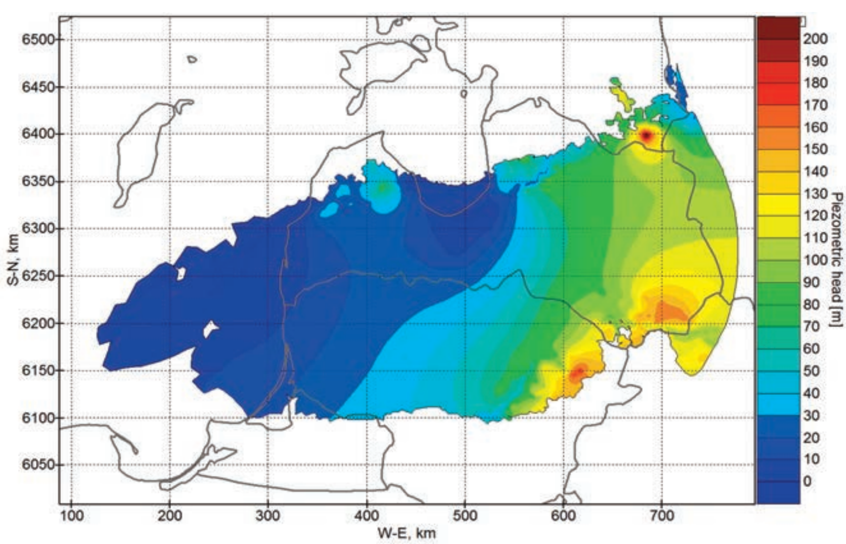

Figure 9. Piezometric head distribution in D3gj layer.

The distribution of piezometric head in a vertical cross-section along line CD is shown in Fig. 10 (see Fig. 8 for the location of line). In the deepest part (Cm layer) transit flow from the southeastern to the northwestern side of the BAB exists, and in most areas it is well isolated from other layers by the Silurian-Ordovician aquitard. The upper aquifers in the active groundwater exchange zones are divided by several thin aquitards and the groundwater flows in these layers are more interconnected. It can be seen that the main recharge area with high head is on the left side of the graph (south-east of the BAB, point C) whilst the discharge areas are in the Gulf of Riga (middle part of graph) and on the right side of the graph (North of the BAB). The flow structure in the upper aquifers has more local character.

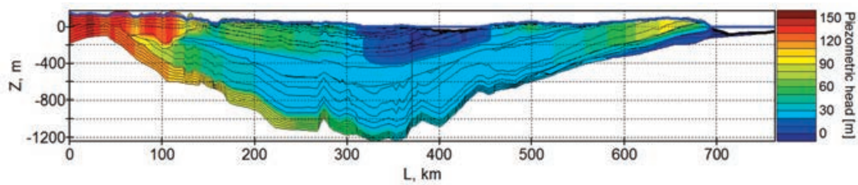

Figure 10. Piezometric head [m] in vertical cross section along line CD (see Fig. 8 for location).

Flow budget and integral parameters

Integrating the flow through the boundaries between individual layers allows the calculation and analysis of the flow balance. Besides the integral over the whole surface, which shows the water abstraction in a particular layer or numerical error, the integrals of inflowing and outgoing flows through each surface are built. The total recharge through the earth (and sea) surface is 5.365e8 m^3/day, the discharge is 5.361e8 m^3/day and the water abstraction is 3.6e5 m^3/day. The misbalance of these numbers is a numerical error and it is 0.02% of the recharge value. The water abstraction is 0.1% of the total recharge in the BAB, however, this ratio should be considered in context, that most of the recharge and discharge takes place in the upper Q layer and only a small part of this water circulates in deeper layers where most of the water abstraction takes place. Additionally, not all wells are included in the model. The inflow through the sub-Quaternary surface to the sub-Quaternary layers is 4.81e7 m^3/day and the outflow is 4.78e7 m^3/day, so the circulation of water through this surface is considerably smaller than through the earth's surface and the water abstraction in sub-Quaternary layers is 0.5% of the inflow. Taking together all Devonian layers the total inflow through the Devonian boundary is 3.6e6 m^3/day, the outflow is 3.5e6 m^3/day and the total water abstraction in Devonian layers is 5% from the inflow value. In the Cm-V layer group, the deepest aquifers, the inflow and outflow integrals are 8.7e5 m^3/day.

The flow budget between groups of layers is shown in table 4. The whole integral flow through the surface, which is equal to the water abstraction of 365e3 m^3/day, goes to the Quaternary layer. The sum of column Q is -263e3 m3/day and this amount is the flow budget which goes to the sub-quaternary layers and is abstracted there.

Table 4. Flow budget 10^3 m^3/day in BAB, divided in 7 layer groups.

from> to	Q	K-C	D23	D2Nr	D12	S-O	Cm-V
Q		126	216	-105	-76	129	-27
K-C	-126		62	0	14	37	9
D23	-216	-62		116	-4	0	0
D2Nr	105	0	-116		5	4	0
D12	76	-14	4	-5		-61	0
S-O	-129	-37	0	-4	61		56
Cm-V	27	-9	0	0	0	-56	

Groundwater flow in the Baltic Sea area in the upper, active water exchange zone is directed from the land into the Baltic Sea, and, according to our results, discharge occurs mainly in the coastal area. The total discharge flow through the vertical plane into the Baltic Sea area is 3.5e6 m^3/day.

Conclusions

The fully script based MOSYS modelling system for generating a geometric model of a geological structure and for the modelling of groundwater flow is developed based on the Python programming language. The system has three basic parts – the information base, the geometry model and the hydrogeological model. Developed high level subroutines allow efficient and repeatable generation of geological structures and the achievement of modelling results.

The capabilities of the modelling system are demonstrated based on the case of the BAB. The results demonstrate that generally the groundwater flow is directed from southeast to northwest, but the shallower aquifers show the strong influence of the local topography.

Acknowledgements

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Groundwater flow beneath the Scandinavian ice sheet in the Baltic Basin

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Abstract

In the last decades it has been shown that most large ice sheets tend to reside on warm beds even in harsh climatic conditions and subglacial melting occurs due to geothermal heat flow and the deformation heat of the ice flow. However, the processes of meltwater intrusion and subglacial groundwater flow conditions have been addressed in only a few studies.

The glacial origin of groundwater in the Cambrian – Eidacaran (Vendian) aquifer system (CAS) in the NE Baltic Basin has been reported on already in the 1980's and supported by oxygen stable isotope studies.

The aim of this study was to establish the groundwater flow pattern in the Baltic Basin (BB) below the Scandinavian ice sheet during the Late Weichselian glaciation. Ice thickness distribution and the topography of the present relief below the ice sheet were used for the ice sheet representation.

Two forcing scenarios were chosen to simulate glacial meltwater intrusion and groundwater flow below the ice sheet – constant head and constant flux approaches.

All of the simulation results suggest reverse groundwater flow direction in the CAS, as well as increased groundwater flow velocities. Particle tracing analysis suggests that meltwater intrusion did not penetrate deeper than 600 m during the last glacial cycle, suggesting that the present distribution of groundwater originating from glacial meltwater is a product of multiple glacial cycles.

Keywords: Baltic Basin; groundwater flow; Scandinavian Ice sheet; glacial meltwater intrusion

Introduction

In the last decades it has been shown that most large ice sheets tend to reside on warm beds even in harsh climatic conditions and subglacial melting occurs due to geothermal heat flow and the deformation heat of the ice flow. However, the processes of meltwater intrusion and subglacial groundwater flow conditions have been addressed in only a few studies.

The Baltic Basin extends over the whole territory of Estonia, Latvia, Lithuania and the Kaliningrad region of Russia, partly to the Leningrad and Pskov regions of Russia, Belarus and the north-eastern part of Poland, as well as wide areas of the Baltic Sea including Gotland Island (Fig. 1)

The glacial origin of the groundwater in the Cambrian – Eidacaran (Vendian) aquifer system (CAS) in the Baltic Basin, particularly in north Estonia, was already reported in the 1980's, supported by the oxygen stable isotope studies (Punning et al., 1987; Vaikmäe et al., 2001).

In recent years, the age constraints of the groundwater in the CAS support glacial meltwater origin, suggesting that at least in the north-western part of Estonia, the groundwater was recharged during the last glacial cycle (Vaikmäe et al., 2001).

However, the extent and therefore the possible volume of the glacial meltwater recharge into the CAS is poorly constrained and groundwater age is poorly understood.

The aim of this study was to establish the groundwater flow pattern in the Baltic Basin (BB) below the Scandinavian ice sheet during the Late Weichselian glaciation. The calculation results were compared with the known distribution of the groundwater body of glacial origin found in the Cambrian – Vendian aquifer in northern Estonia which is believed to have originated as a result of subglacial meltwater infiltration during the reoccurring glaciations.

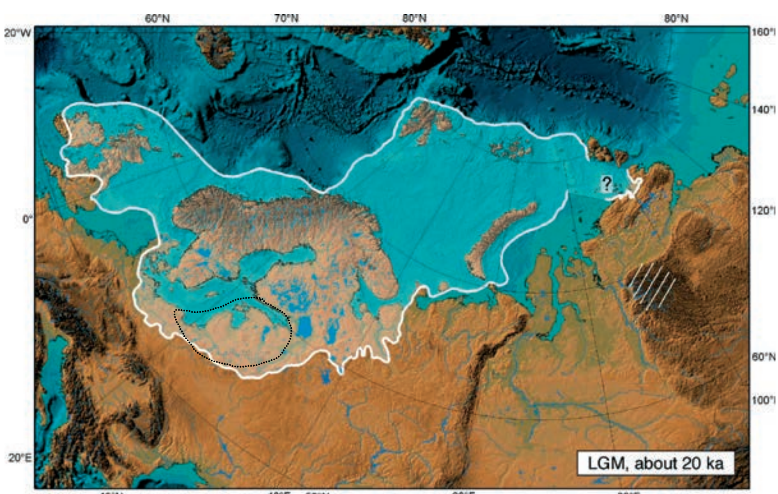

Figure 1. The extent of the Scandinavian Ice Sheet during the Last Glacial Maximum (After Svedsen et. al., 2004) and position of the BB (black line).

The geology of the Baltic Basin

The geological structure of the Baltic Basin is given in detail in section I of the current issue. Therefore, in this section we will emphasize the general framework of the aquifer – aquitard system.

An overview of the hydraulic properties and stratigraphy of the BB is given in figure 2. The Baltic Basin in general can be subdivided into three aquifer systems: the Upper Devonian, the Lower Devonian and the CAS respectively (Fig. 2).

	Layer	Hydraulic properties	Description
Q	Quaternary	aquifer	Quaternary deposits
Q2	Quaternary	aquitard	
Q3	Quaternary	aquifer	
Q4	Quaternary	aquitard	
PgNg	Paleogene - Neogene	aquifer	Local
K	Cretecious	aquifer	SE part of the BB
J	Upper Jurassic	aquitard	SE part of the BB
J*	Lower Jurassic	aquifer	SE part of the BB
T	Triassic	aquitard	SE part of the BB
P2	Upper Permian	aquitard	SE part of the BB
P2*	Lower Permian	aquifer	SE part of the BB
C	Upper Carboniferous	aquifer	Upper Devonian active water exchange zone. Numerous aquitards are very thin, therefore only of local importance
C*	Lower Carboniferous	aquitard	
D3jnsk	**D3 Jonishku - Shkervela Fms**	aquifer	
D3stel	D3 Stipinu - Elejas Fms	aquitard	
D3ogkt	D3 Ogres - Katleshu Fms	aquifer	
D3ogkt*	D3 Ogres - Katleshu Fms	aquitard	
D3dg	D3 Daugava Fm	aquifer	
D3slp	D3 Salaspils Fm	aquitard	
D3pl	D3 Plavinas Fm	aquifer	
D3pl*	D3 Plavinas Fm	aquitard	
D3am	D3 Amata Fm	aquifer	
D3am*	D3 Amata Fm	aquitard	
D3gj	D3 Gauja Fm	aquifer	
D3gj*	D3 Gauja Fm	aquitard	
D2br	D2 Burtnieku Fm	aquifer	
D2br*	D2 Burtnieku Fm	aquitard	
D2ar	D2 Arukila Fm	aquifer	
D2nr	D2 Narva Fm	aquitard	Regional aquitard
D1gr-D2rzpr	D1 Garzhdu - Pernava Fm	aquifer	Lower Devonian aquifer system
S4pr	Pridolian	aquitard	Silurian - Ordovician regional aquitard - Stagnant water exchange zone except in N Estonia
S3ld	Ludlovian	aquitard	
S2vn	Wenlockian	aquitard	
S1ln	Llandoverian	aquitard	
O3	Late Ordovician	aquitard	
O2	Middle Ordovician	aquitard	
O1	Early Ordovician	aquitard	
Cmtr	Cambrian	aquifer	Cambrian - Eidiacaran aquifer system (CAS) - Stagnant water exchange zone except in N Estonia and SE Lithuania
Cmln	Cambrian Lontova Fm	aquitard	
V2vr	Eidiacaran	aquifer	
V2kt	Eidiacaran	aquifer - aquitard	
V2gd	Eidiacaran	aquifer	

Figure 2. Model layers and there equivalent stratigraphic units.

The relief of the Baltic Basin was shaped by the preceding glaciations (except the area of the Baltic Sea) and therefore Quaternary sediments, mostly of glacial origin, cover the sedimentary sequence of the BB. In parts Quaternary sediments can reach significant thicknesses (mostly in highland areas, characterized by glacier deposition (Zelčs et al., 2011; Kalm et al., 2011; Guobyte and Satkūnas, 2011) and some depressions) and can store an important volume of groundwater on a local scale.

The Middle and Upper Devonian aquifers and aquitard system lie above the Narva regional aquitard. Most of these are only of sub-regional extent as the distribution of this system is rather uneven. Permian to Cretaceous sediments occupy a large portion of the BB in the W and SW.

All of these sub-regional aquifers are considered in this work as the upper aquifer system of the BB, which can be regarded as an active water exchange zone, and in general make up the upper 200 to 300 m.

The extent of the middle Devonian Narva aquitard more or less coincides with the extent of the D1-2 aquifer system. This unit is composed predominantly of marls and clays, but in the NE some areas of this unit are composed of sandstones with aquifer properties.

The lower Devonian aquifer system (D1-2) occupies the eastern and central parts of the BB, but in most of the Baltic Sea territory it was eroded during the Carboniferous (Kuršs, 1992). It is composed predominantly of sandstones, with some admixture of siltstones, marls and clays and reaches a thickness of 200 m in the western end.

Below the lower Devonian aquifer system lies the Ordovician - Silurian (O-S) aquitard, which is composed of predominantly marls, dolomitic marls, clays and argilitic clays with occasional limestone and dolostone beds. In the very NE of the BB, near the earth's surface, this unit is more an aquifer than an aquitard but as this unit plunges towards the SW, the carbonatic rocks display more aquitard properties, suggesting a decrease in conductivity due to the burial depth. In a study by Perens (1984), Perens and Paltanavičius (1989) and Perens et al. (1994) it has been shown that at depths greater than 100 m this unit displays aquitard properties.

The CAS covers the crystalline basement and is composed mostly of sandstones, siltstones and clays. The thickness of this aquifer system changes from 50 – 200 m, and it plunges from up to 50 m a.s.l. elevation in the NE and SE of the basin to -5000 m b.s.l. in the SW. In the upper limits in the NE this unit is an active water exchange aquifer system (Vallner, 2003; Raukas and Teedumäe, 1997) and groundwater is used for water supply. In the central and moreover eastern extent of the aquifer system, where it is generally buried below sedimentary rocks -2000 m b.s.l., groundwater salinity increases to brine and abnormal pressure heads have been reported from SW Lithuania, suggesting slow or stagnant groundwater (Mokrik, 1997; Zuzevičius, 2010).

The Quaternary history of the BB: warm stages, permafrost and glaciations

During the Quaternary, the Baltic Basin was glaciated at least 4 times (Kalm et. al., 2011; Zelčs et. al., 2012, Ehlers, 1991). Marine isotope stages (ibid) and other proxy data suggest the existence of significantly more glacial advances during the Quaternary than are preserved in the geological record. However, most of the evidence for the presence of ice sheets is available from the last Weichselian glaciation (Kalm et. al., 2011; Zelčs et. al., 2012; Guobyte and Satkūnas, 2011, Ehlers, 1991). The extent of the Saalian and Elsterian ice sheets is signified by the marginal landform assemblage in Eastern and Central Europe (Ehlers et al, 2012; Karabanov & Matveyev, 2012; Matoshko, 2012; Marks, 2012 and many others).

Key variables controlling the volume of glacial meltwater intrusion into the aquifer system, apart from the geological setting, are the duration of the ice cover and development and degradation of permafrost in the subglacial and periglacial settings. However, data is sparse for the first, and almost non-existent for the second, meaning that reasonable assumptions are necessary.

The alternation of the ice age/interglacial conditions denotes that three types of environments with rather different hydrological conditions succeeded each other: (1) Warm stages – Holocene like conditions, (2) cold stages, e.g. periglacial conditions and (3) subglacial conditions.

Conditions during the warm stages were largely similar to modern conditions (e.g. Kloz et al., 2003) and it can be assumed that the groundwater flow pattern was very similar to the pre-industrial Holocene conditions.

During the cold stages, permafrost development effectively led to conservation of the aquifer system, and the upper aquifers were subjected to cryogenic hydrological processes. It can be assumed that during the Weichselian cold, ice free stage (MIS 4 and 3) aquifer recharge by precipitation was at its lowest (Williams, 1970).

During the glacial phase, the Scandinavian Ice Sheet extended over the BB area from N, NE to S, SW (Ehlers, 1993; Svedsen et al., 2004; Zelčs et al., 2012) and retreated in a reverse direction during deglaciation (Kalm et al., 2011). Permafrost thawed under the ice cover due to: (1) insulation of the glacier bed, thus allowing geothermal heat to slowly increase the ground temperature and (2) heat energy generated due to ice and sediment deformation at the glacier sole (Waller et al., 2012). This may result temporarily in the development of unfrozen ground conditions at the ice bed overlaying still frozen ground.

Additional difficulty in the parameterization of glacial hydrology is caused by the presence of subglacial till. Most glaciers overriding soft sediments like those found in the depression of the Baltic Sea are underlined by fine grained basal till. Effectively it acts as an aquitard, but its distribution varies both in time and space (Evans et al., 2006, Piotrowski et al., 2004).

Glacial water in the BB aquifer system

The glacial origin of the groundwater in the CAS of Estonia has been suggested by Punning et al. (1987) and Vaikmäe et al. (2001). Both suggested that glacial meltwater with a more negative σ18O composition intruded into the CAS. The noble gas analyses (Vaikmäe et al., 2001) allowed the conclusion that palaeorecharge took place at temperatures around freezing point.

The exact process of intrusion is still under discussion. Jõeleht (1998) suggested that intrusion took place through the aquifer outcrop area in northern Estonia while Mokrik (1997) suggested that the depleted stable isotope composition of oxygen was a result of cryogenic processes under permafrost conditions.

The calculated groundwater residence time by the ^{14}C method suggests an age between 12,000 and 25,000 radiocarbon years, which corresponds to the existence of the Weichselian ice shield in Estonian territory (Raidla 2010, 2012). Although Raidla (2010) also concludes, that the important differences in residence times appearing between samples from west-Estonia and from the rest of the research area are probably caused by different infiltration mechanisms.

In the latest investigations the process of intrusion of meltwater is favoured (Marandi, 2007, Vaikmäe et al., 2008, Raidla et al., 2009) although there is no support from hydrodynamic modelling so far. Therefore, the extent and possible volume of the glacial meltwater recharge into the CAS is poorly constrained as is the groundwater age distribution.

The model setup

The geometry model of the BB geological structure and groundwater conductivities of the aquifers and aquitards were used from the PUMA V1 groundwater flow model (Virbulis et al., 2012, this volume).

A 3D Darcy flow with free-surface and anisotropic conductivity is assumed for the steady state model runs:

$$\frac{\partial}{\partial x}\left(K_{xy}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{xy}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial z}\left(K_{z}\frac{\partial h}{\partial z}\right)+Q=0 \quad (1),$$

where h is the piezometric head, Q are the sources of water abstraction and K_{xy} and K_z are the horizontal and vertical hydraulic conductivities.

The position of the free surface is assumed equal with the calculated head h. As all, except Quaternary, units are confined and only a small part of the Quaternary unit itself is unconfined in the ice free area, the conductivities are not adapted according to the water content in the element as often used for unconfined aquifers, McDonald (1989).

The Finite Element (FE) method with Galerkin weighted residuals is used for solving the equation. A detailed description of the hydrogeological model used is given in Virbulis et al. (*in print*) and this volume.

During the formation of the global FE matrix only non-zero elements and a connection matrix are created. The matrix is solved using direct sparse solver PARDISO, Schenk (2006).

The Precambrian basement forms the impermeable lower boundary of the model as suggested by Levins et al. (1998) and Mokrik (1997). On the northern and western side of the BAB, the basement reaches the earth surface and the thickness of the model is zero. On the south-western side the BB borders the Danish-Polish basin with a zone of extensive faulting and this boundary is assumed as impermeable following Mokrik (1997). The eastern side of the BB is connected with the Moscow Artesian Basin and the south-eastern boundary is the Belarus-Masurian anticline. The thickness of the BB at these boundaries is approximately 300 – 500 m. Zero water exchange (no flow) is assumed through these boundaries.

For the glacial forcing, the Ice 6G model was applied. It is a physical model developed in the University of Toronto Glacial Systems Model (GSM) (Argus, 2010). The GSM is a physically based model, employing a shallow ice approximation whereby the vertical length scale is much smaller than the horizontal length scale. The model is subject to the equations of conservation of mass, momentum, and internal energy, represented as a set of nonlinear coupled diffusion equations in essentially two dimensions, applied to a spherical Earth. A detailed description of the equations and model development can be found in Deblonde and Peltier (1991, 1993), and more recently in Tarasov and Peltier (1997, 1999, 2005). Various model outputs include normal stress on the ground surface caused by an ice-sheet, permafrost depth, basal temperature relative to the pressure melting point of ice, surface lake depth, basal meltwater production, basal surface elevation subject to isostatic adjustment, surface elevation of ice-sheet, and ice-sheet thickness.

Two data sets from Argus (2010) were used – the correction for the topography due to the glacioisostatic loading and the ice thickness distribution over the study area during the last glaciation. The datasets were subdivided into 19 different ice thicknesses and corresponding topography adjustment scenarios, covering the time span from 28 – 10 ka BP.

It has been shown that the water conductivity of carbonate rocks is highly sensitive to lithostatic pressure (Perens, 1984), mostly due to the fact that the largest portion of the groundwater transport through carbonate rocks occurs along the joint and fracture network. Increasing lithostatic pressure, along with the increasing depth, forces a decrease in the joint and fracture aperture, as well as disrupting the connectivity network, and some critical depth (usually of the order of 100 m, or where lithostatic pressure reaches values 10^5 kPa) groundwater flow is restricted to filtration through the pores, which is at least a 2 to 3 orders of magnitude slower process. Contrastingly, sandstones are not as sensitive to the changes in lithostatic pressures. In this study, we have estimated a decrease in porosity due to the applied vertical glacier stress, following the calculation procedure, as shown by (Zimmerman, 1991). The results suggest, assuming elastic rock behaviour, that the porosity change in the Cambrian aquifer is expected to be of the order of 1%. Given that the measured porosity for the Cambrian aquifers is on average 20%, this change is insignificant, and was ignored in the numerical simulations.

A simple depth dependant model was used to correct the water conductivities of the carbonitic aquifers to better reflect the effects of the glacial loading to the carbonate aquifers, as described in (Perens, 1984). Five aquifer water conductivities were adjusted according to the formula (I)

$$K_{xycond}=K_{xy}*(100-h)/100$$

where K_{xycond} – depth adjusted water conductivity; K_{xy} – water conductivity of the aquifer unit near surface, h – depth.

Further, several simplifications and assumptions were made to the model: the ice sheet was considered to be in a temperate state; no permafrost was considered in the study area; no adjustment of the Quaternary cover; no fluid density gradients considered for different water bodies.

Two sets of boundary conditions below ice were used to model the recharge effects from the glacier into the aquifer system: constant head and constant flux.

A constant head boundary condition was defined as the water pressure equivalent to the overlying ice thickness. This is considered as a critical scenario as it has been shown that the Scandinavian Ice Sheet bed conditions were not temperate along the whole ice/bed boundary in space and in time (Kleman & Bögstrom, 1994), even though this assumption gives the estimate of the maximal possible pressure heads at the glacier base under given ice thickness scenarios.

As a more realistic approach, a constant flux boundary condition was chosen. It has been estimated that the meltwater production at the glacier bed due to the geothermal heat flux, shear heating as well as infiltration of the meltwater from the glacier surface and interior is of the order of millimetres per year per square meter (Cuffey and Patterson, 2010). However, modelling results suggest that only a tiny fraction of this water is recharged into groundwater and so by far the biggest portion is transferred to the glacier margin through englacial and subglacial conduits (R and N channels) as well as sheet flow as suggested by (Boulton et al., 2007 a and b). The constant flux boundary condition had to satisfy the ice sheet stability condition – the pressure head generated by the constant flux cannot exceed the elevation of the ice sheet except under the ice streams (Cuffey and Patterson, 2010) which make up a small fraction of the ice sheet (Cuffey and Patterson, 2010). Iterative studies suggested that only constant fluxes as low as 2X10-5 – 10-6 mm/m^2 satisfied this condition and in these cases the .pressure head at the glacier was close to the glacier surface.

Results

Constant head simulations

The constant head simulations were carried out assuming that the head at the glacier base is equal to the overlying ice thickness. This was considered as a scenario simulating the highest possible pressure heads generated below the glacier.

Simulations suggest reverse groundwater flow in the whole BB as compared to the present day state. In all aquifers equipotential lines reflect the distribution of the ice thickness, except those in the CAS, where due to complete disconnection by faults, areas of comparable low pressures remained through the glaciation (Fig. 3 B and D). By comparing this to the pre-industrial groundwater flow (Fig. 3 A), almost all of the BB is over-pressurized for at least 12 ky.

The calculated groundwater flow velocities, along with pore pressure, increase under subglacial conditions, though the increase is spatially different. Figure 3 C and D illustrate velocity modulus for the Eidicaran V2gd layer aquifer under "interglacial" conditions. The "interglacial" scenario simulation is based on the Baltic Artesian Basin groundwater flow model (Virbulis et al., *accepted for publication* and Virbulis et al., *this volume*) not without water abstraction. The V2gd aquifer was chosen as an illustration of the groundwater flow velocity change in the deep aquifers. The highest velocities under the interglacial scenario occur along the aquifer discharge area (Fig. 3 C) while the highest velocities in the subglacial scenarios occur along the glacier margin (Fig. 3 D). The velocities in the CAS in general increase in the eastern, shallower part of the basin, while the velocity change is negligible deeper than approximately 1,000 m.

The calculations suggest two main recharge zones for the CAS (Fig. 3 B and D). The areas remained active for 12 ka and under the current model setup are the main sources of the glacial meltwater intruded into the CAS.

Constant flux simulations

A constant flux scenario was viewed as a more realistic way of simulating meltwater recharge into the aquifer system. Constant flux was set to 1e-5 m^3 per m^2, as in the case with higher flux values, pressure heads beneath the ice would greatly exceed the ice elevation – an unstable condition considered as unrealistic (Lemieux et al. 2008). This scenario is considered as a best modelling approach under current data sets and will be explored below. A similar approach was used in the work of (Lemieux et al. 2008 a,b,c) setting the conditions that the water pressure cannot exceed that of the covering ice as a stability condition.

The calculation results show the same groundwater flow directions in the aquifer system, as in the constant head scenario while pressure head distribution in this case is in general lower (Fig. 3 E, F and G). Pressure head distribution under the given simulation yields over the pressured area in the Baltic Sea area adjacent to Swedish coast. This area, according to ICE 6G has lower ice elevations and coincides with the Baltic Ice Stream (Kleman & Glaser, 2007).

The recharge of the glacial meltwater into the CAS presumably occurred along the northern extent of the CAS, where it is reaching the earth surface, and presently outcropping along the Estonian northern coast. As a potential recharge zone it is deduced from the distribution of the dO16/18 ratio in the groundwater, where it has the ost negative values in the very NE and NW of Estonia (Raidla, Mokrik). Both modelling scenarios confirm this assumption.

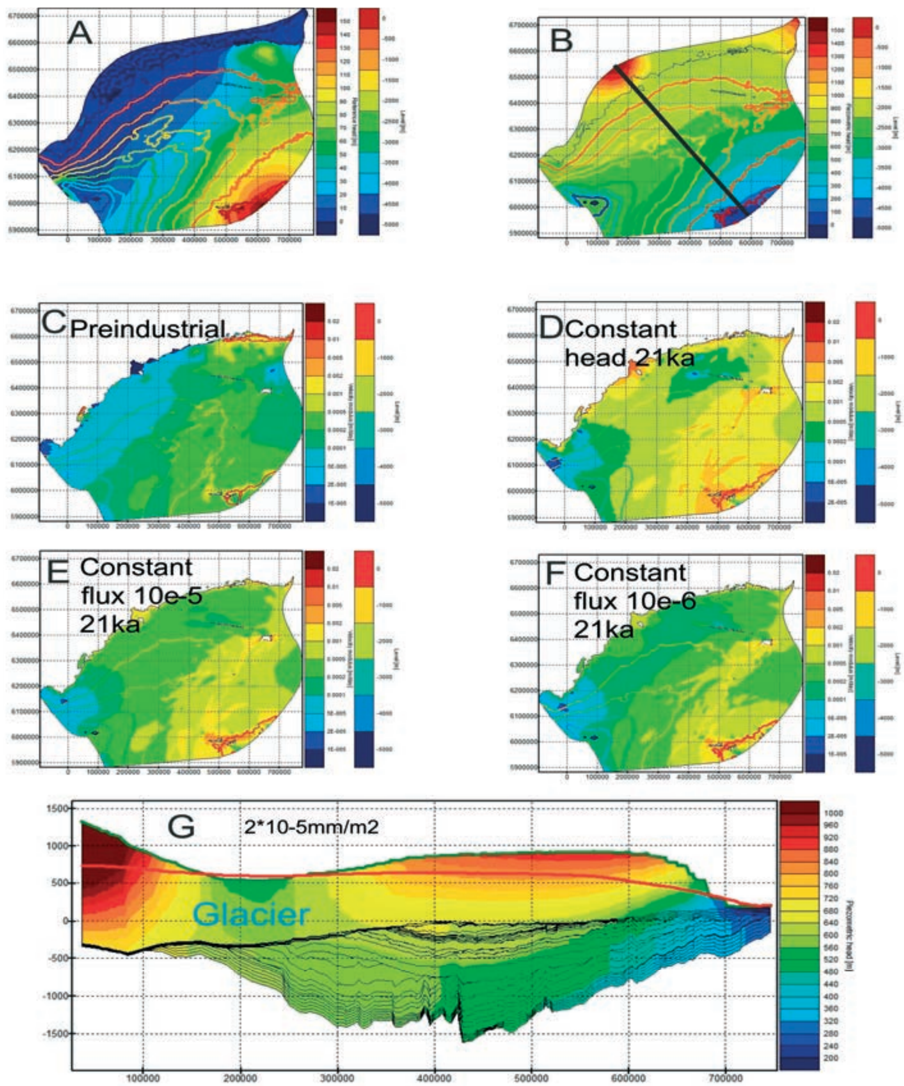

Figure 3. Comparison between subglacial and interglacial hydraulic conditions. For subglacial conditions ICE 6G 21ka scenario is shown. A – Preindustrial (Interglacial) scenario piezometric head distribution in the CAS; B – Piezometric head distribution in the CAS Constant head scenario; C – Preindustrial (Interglacial) velocity modulus distribution in the CAS (Layer V2gd); D - Piezometric head distribution in the CAS (Layer V2gd) Constant head scenario; C – Preindustrial (Interglacial) velocity modulus distribution in the CAS (Layer V2gd); D – Constant head scenario velocity modulus distribution in the CAS (Layer V2gd); E - Constant flux (flux=2*10E-5 mm/m^2) scenario velocity modulus distribution in the CAS (Layer V2gd); F - Constant flux (flux=2*10E-6 mm/m^2) scenario velocity modulus distribution in the CAS (Layer V2gd); G – Cross section along the line in figure B showing piezometric head distribution in the BB. Red line depicts the hydraulic pressure along the ice/bed interface.

As in the case of constant head simulations, the recharge areas for the Cambrian aquifer system are placed in the NE and NW of the BB, and the NW is a more important one. This is governed by the geology of the BB: recharge areas coincide with areas where the Cambrian aquifer system is outcropping through the Quaternary cover, Quaternary sediments in this area in general are quite thin and predominantly composed of sandy facies; secondly, an even better pronounced intrusion area is situated at the NW corner of the BB. Its presence here is controlled by the Lontova aquitard (Cmln) distribution, where it is composed of clay and thicker in the Eastern part, and silty and thinner in the western part (Vallner, 2003; Raukas and Teedumäe, 1997).

Meltwater intrusion depth

Particle tracing analysis was carried out in order to quantify the glacier meltwater intruded into the aquifer system. Particle tracing was carried out by employing a paraview 3.14.1 software particle tracing calculation module. The particles were calculated as a function of calculated velocity modulus (porosity assumed to be 20% for all the geological structure) and time. The results are presented as a depth isoline map showing the depth that meltwater intruded during the simulation runs. The model predictions suggest that meltwater intrusion into the Cambrian aquifer does not exceed a depth of 400 m, while along most of the CAS northern border intrusion it does not propagate more than 200 – 300 m (Fig. 4).

Meltwater intrusion into the lower Devonian aquifer system, as is the case with the CAS, is generally spread along the layer sequence northern outcropping line (Fig. 4) of the CAS. Also, the intrusion is more pronounced in the NW, which is predefined by the geological structure. Similarly to the CAS, the groundwater flow is directed from N to S in this aquifer system (Fig. 4).

The simulation results also predict that most of the groundwater in the upper Devonian aquifer system in Estonia, Latvia and E Lithuania, excluding SW Latvia and E Lithuania, was replaced by glacial meltwater during glacial periods. The calculation shows that an even up to 400 m deep intrusion of meltwater occurred into the Cretecious aquifer in the SW district of the BB (Fig. 4).

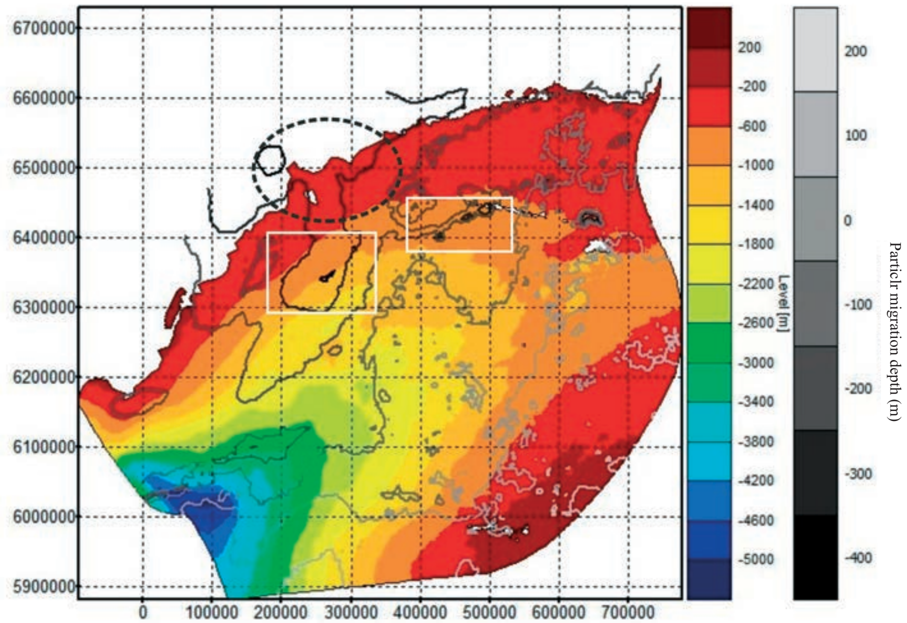

Figure 4. The depth of the glacial meltwater intrusion (grey scale bar) into the BAB. Black dotted line ellipse denotes the area of the meltwater intrusion into the CAS, white line rectangles denote meltwater intrusion area into the Lower Devonian aquifers.

Discussion

Verification of the results

C^{14} datings of groundwater, $\delta^{18}O$ value for groundwater and geochemistry of groundwater in N Estonia allowed for the proving of glacial meltwater origin for the freshwater in the aquifer (Vaikmäe et al., 2008). Unfortunately, this data is predominantly distributed along the coastal area and isotope data is sparse further south. Likewise, the available groundwater age datings using the ^{14}C method cover the area in northern Estonia (Raidla, 2010) and Lithuania (Mokrik et al., 2008) while there is no such data in the territory in between. The suggested age of isotopically light groundwater in northern Estonia is between 12 and 20 thousand years (Raidla, 2010) proving late-glacial origin. These data are bound to the northernmost strip of the Cambrian-Vendian aquifer. Whether the isotopically light groundwater found further to the south is of late-glacial origin or preserved from earlier glacial advances is not clear. However, the model analysis suggest that more than one glaciation is needed to produce the volume of meltwater preserved in the Cambrian-Vendian aquifer.

The composition of the groundwater in the Cm aquifer system in Latvia and Lithuania is profoundly different from that observed in northern Estonia, suggesting a different age and origin of this groundwater body. However, groundwater of rather high mineralization is found in the rocks of the crystalline basement even in the north of Estonia (Karro et al., 2004). Additionally, occasionally observed relatively high chloride concentrations and Na to Cl ratios above one (Raidla et al., 2009) can be interpreted as the result of geologically recent saltwater replacement with freshwater.

So, it can be speculated that prior to the Quaternary glaciation brine found in the Cambrian aquifer was present up to its northern limit of distribution.

The groundwater age datings in Lithuania consider the Devonian rather than the Cambrian aquifer. The reported groundwater age is up to 30 thousand years (Mokrik et al., 2008). However, the stable isotope data does not suggest the presence of any significant amount of glacial meltwater – observed $\delta^{18}O$ values are close and even above modern precipitation values for the deepest part of the basin.

Geochemical $\delta^{18}O$ isotopical data allows for the drawing of a line in the Cm aquifer system separating groundwater with a probable admixture of glacial meltwater and one – without. The modelled meltwater intrusion for a single glacial period was not able to reach this line, and even by increasing the recharge time 10X the model predicts only some 50% of the area occupied by the glacier meltwater within the Cm aquifer.

In our opinion, there are two major factors contributing to this problem. First – the Quaternary sediment conductivity beneath the ice sheet is one of the limiting factors in regulating how much of the meltwater will reach the aquifers beneath these sediments. In the current model setup Quaternary sediment vertical conductivities were the same as for the modern day setup. In this setup, all of the Baltic Sea bed is covered by low conductivity clay sediments, which also cover the Cm aquifer in its northern outcropping area. However, it can be suspected that under subglacial conditions these sediments became rapidly eroded and the Cm aquifer system was directly exposed to the ice bed. To test this, we did a simulation set with changed uniform vertical and horizontal conductivities of the Quaternary sequence set to 10 m/day. As a result, the depth of the meltwater intrusion increased, however, not too much (Fig. 5).

Secondly, it has been shown that paleoincisions can increase the vertical connectivity of the aquifers in northern Estonia (Marandi et al., 2012). In this study, model resolution did not allow the accommodation of paleoincisions. Incision in the Prequaternary surface filled with ice or glaciofluvial sediments would enlarge the outcrop area available for subglacial meltwater infiltration thus facilitating the subglacial groundwater recharge.

Groundwater flow beneath an ice sheet

As has been indicated in previous studies, the ice-bed interface is the major router of the meltwater while meltwater transferred into the aquifer system constitutes only a small portion of the groundwater (Shoemaker, 1986). Our simulations suggest that meltwater intrusion into the aquifer system is a 5 order smaller amount of what's being melted from the glacier. Overall, aquifers are ineffective media for subglacial meltwater drainage. Simulated meltwater intrusion does not penetrate a depth over 600 m, in the case of the CAS. On the other hand, the model predicts that most of the groundwater in the upper Devonian aquifers during the glacial advance was replaced by meltwater, and preglacial groundwater remains only at depths below -200 m b.s.l. (Fig. 5). Therefore, the geological setting of the aquifers and aquitards seems to set the main controls over the depth and amount of meltwater intrusion. The Upper Devonian aquifers are well exposed on the surface, while the Lower Devonian and the CAS are outcropping over a narrow belt, and the area of the intrusion is limited. Secondly, the thickness of the Lower Devonian and the CAS increase in the southern direction resulting in a dispersion of the meltwater intruded.

The dual approach of the boundary conditions used as glacier forcing was used. Even though the results obtained generally show the same picture, second order differences can be picked up. The ice thickness approach (the head at the glacier sole is equal to the weight of the overlying glacier) in general gives higher pressure heads, and higher pressure gradients especially along the ice sheet margin, where the glacier ice tends to be very steep (Argus, 2010). Particle analysis of the ice thickness scenario also suggests deeper glacier meltwater intrusion into the Cm aquifer system.

The constant flux approach, however, in general, results in the pressure head at the glacier sole being more evenly distributed, with approximately 10% less pressure head on the average, than in the constant head scenarios.

In order to characterise the groundwater transport, transient analysis is needed, especially for the deep aquifer systems.

Effects of a fault on groundwater flow

The groundwater flow in the upper aquifers, as was expected, is governed by the distribution of ice sheet thickness and a N, NW-S, SE pressure head gradient is present throughout the geometry. However, more complicated patterns can be recognized in the deep CAS.

The Caledonian stage sediments have been faulted, and in many places the CAS is disrupted and disconnected for more than 50 km (see section 2). This has a profound effect on the pressure head distribution in the CAS (Fig. 3 G).

It has been suggested that some areas in the CAS bear abnormally high pressures, which could not be explained by topographical effects (Mokrik, 1997; Zuzevičius, 2010), while measurements in the O-S aquitard indicate abnormally low pressures.

Modelling results suggest that during subglacial conditions these areas in the CAS are under-pressured compared to the rest of the aquifer, due to a shielding effect by the translated strata. Coincidentally, these patches are the ones, in which abnormally high pressures have been reported (Zuzevicius, 2010).

Conclusions

The model simulations allow one to draw conclusions on several aspects of the long term groundwater dynamics in the BB:

A constant flux boundary condition on the glacier bed, in our view, is a more realistic representation of the subglacial hydraulics as the volume of meltwater intruded into the aquifer system can be controlled by the pressure head.

The aquifer system is able to accept only a tiny fraction of the volume of meltwater produced in the subglacial setting.

The BB aquifer system has been replenished by glacial meltwater, and it penetrated up to 200 m deep into the deepest aquifer system. However, to explain the wide occurrence of glacial origin groundwater in northern Estonia, multiple glaciation scenarios have to be considered.

The presence of glacial, low conductivity sediments at the glacier bed is one of the major controls on the volume which can be intruded into the aquifer system.

Transient analysis is needed to establish the groundwater dynamics of the deepest aquifer/aquitard systems during the glaciation phase.

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A list of the factors controlling groundwater composition in the Baltic Artesian Basin

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Abstract

The chemical composition of groundwater is the result of long term interaction between rocks and water complicated by the continuous addition of infiltration water and mixing due to dispersion along flow-lines and diffusion. Thus the geological structure determining groundwater flow and rock composition itself controls the trends of groundwater chemical evolution. A list of the factors that directly affect the composition of the groundwater within the Baltic Artesian Basin can be drawn: (1) the composition of precipitation and infiltration water as a starting point for the chemical evolution and the almost immediate weathering of carbonate minerals in reactions with carbon dioxide derived from the atmosphere and soil; (2) oxidation- reduction systems controlled by the presence of dissolved oxygen and organic matter in a dissolved or solid state that affect the mobilisation of the reduced forms of sulphur, iron and manganese in the groundwater; (3) the dissolution of gypsum and halite found in some parts of the basin adds calcium, magnesium, sulphate sodium and chlorine ions to the solution; (4) the presence of formation brines and the evolution of their composition during geological time and (5) anthropogenic influences that can range from changing flow patterns in areas of intensive water abstraction to the changing composition of infiltration water in agricultural and urban territories.

Keywords: Baltic basin, hydrogeochemistry, groundwater composition

Introduction

The chemical composition of groundwater is the result of long term interaction between rocks and water complicated by the continuous addition of infiltration water and mixing due to dispersion and diffusion. Thus both the geological structure determining groundwater flow and rock composition itself controls the trends of groundwater chemical evolution.

The characteristic feature of groundwater composition is vertical zoning (Jodkazis, 1989; Levins, 1990). The freshwater zone (total dissolved solids, TDS up to 1 g/l) where HCO_3-Ca-Mg waters are usually found; The brackish and saltwater zone (TDS 1 to 35 g/l) where Cl-Na to Cl-SO_4-Na-Ca water types are encountered; brines (TDS > 35 g/l) with prevailing Cl-Na or Cl-Na-Ca. It is worth mentioning that from a dynamic point of view, three similar zones – the active water exchange zone, the passive water exchange zone and the stagnation zone – reflecting the speed of exchange are identified as well. Both classifications are spatially overlapping, but not fully. To put it simply, in most cases freshwater is found above the topmost regional aquiclude, brackish water resides below the first regional aquiclude and brines – are found below the second regional aquiclude. Vertical zoning is primarily depth related rather than constrained to specific aquifers and aquitards. However, in several parts of the Baltic Artesian Basin (BAB), zoning can be directly related to the specific geological formations. The greatest depth where freshwater is encountered can vary significantly – from a few meters to 600 or more and this cannot be explained only by modern groundwater flow patterns. Freshwater can be found in the underground regions that are characterised by extremely slow or absent observable groundwater flow.

Given the relatively undisturbed geology of the region, groundwater composition is often associated with the stratigraphical unit it is found in. This might be the case for the local or sub-regional scale; however, it is certainly not true for the whole basin: groundwater salinity increases persistently with increasing depth. However, the salinity increase is not linear: abrupt increasing of the salinity is observed across regional aquicludes like the Lower Triassic, the Narva formation and the buried part of the Ordovician-Silurian complex.

The major anions (Cl^-, SO_4^{2-}, HCO_3^-) and cations (Na^+, K^+, Ca^{2+} and Mg^{2+}) are mainly considered in this paper. Most groundwater composition classifications indicate the three basic types according to the dominant anion: bicarbonate water, sulphate water or chloride water (Drever, 1997).

Bicarbonate water is the most common freshwater type. Dissolved salts in it are mostly derived from the weathering of carbonate as well as silicate minerals. Calcium and magnesium ions usually make up the bulk of cations in this water type.

Sulphate water is usually derived from the dissolution of gypsum. Calcium and magnesium are the dominant anions here. Magnesium is derived from the dedolomitization reaction that consumes dolomite and calcium ions and produces calcite, and releases magnesium ions into the solution. Another source of sulphate can be the oxidation of pyrite or other sulphide minerals. Given the prevalence of carbonates in the sedimentary cover, the result of this process will be very similar to gypsum dissolution, however, the sulphate concentrations may not reach such high levels.

Water with chloride as the dominant cations is usually derived directly or indirectly from sea water. Very strong brines can be produced with a TDS of more than 300 g/l (e.g. Bukaty, 2009; Davisson and Criss, 1996) as a result of seawater evaporation or dissolution of evaporite sediments, that themselves have usually originated from sea water in the geological past. For the strongest brines, Na as the dominant cation is often replaced with Ca and in extreme cases with Mg. The dilution of strong brines obviously can introduce corrections to this general trend. Cl-Na, Cl-Na-Ca and Cl-Ca-Na brines with different concentrations are found within the BAB.

Groundwater formed in rather different paleoclimatical settings is expected to reside even in the active water exchange zone. The active water exchange zone hosting mostly freshwater can be up to 600 m (Jodkazis, 1989) thick. According to hydrogeological models (Virbulis et al., 2012), the distance from recharge to drainage regions can be more than 200 km with a modelled flow rate in the order of 10^{-3} to 10^{-4} m/day, e.g. in the Arukila formation, the flow passes from South-East Latvia to the Gulf of Riga. Obviously the water residence time should be at least several tens of thousands of years. This is a time span stretching well into the Pleistocene, when advances of Scandinavian glaciations and arctic climatic conditions should have resulted in rather different groundwater flow patterns. Thus, the recharge conditions of a large volume of the freshwater residing in the BAB cannot be unambiguously identified using present day observations.

Methods

This work is based on a literature review and analysis of the hydrogeochemical data collected in the wells data base maintained by the Latvian Environment, Geology and Meteorology Centre as well as similar records kept by the Lithuanian Geological Survey and the Geological Survey of Estonia. The data set includes many thousands of water analyses completed from as early as 1939 and up to recent observations. Most of the data illustrating water composition from aquifers that are not used for water abstraction are from Soviet times in the 1960's, 1970's and 1980's of the last century (actually until 1991), when extensive geological and hydrogeological mapping campaigns on a scale of 1:200 000 and 1:50 000 were undertaken and oil and gas prospecting took place.

Measurements from wells of disputable quality as well as measurements where the ion balance is not within 5% were excluded from the data analysis.

It should be noted that an evaluation of hydrogeochemical monitoring data in Latvia demonstrated that 4 to 6% of all results of chemical analyses compiled in the data bases seemed to be erroneous (Teterovskis and Kalvāns, 2012). These errors often cannot be identified by simple ion balance analysis, as in the past several parameters were not determined directly, but calculated from indirect indices. Additionally, the ill-treatment of samples, such as freezing which induces precipitation of calcium carbonate, can affect the quality of results as well.

Factors controlling groundwater composition

The evolution of groundwater composition can be traced along a flow line that starts at the recharge area, filters through rocks of different composition and ends in a discharge area that very often is near the shore line above or below the water table. Evaporation and biological processes already change the composition of precipitation water dramatically at the topmost part of the soil and sediments. Bicarbonate water is generated there most often. As the water infiltrates deeper, the oxygen and organic compounds derived from the soil are used up to fuel water-rock reactions that usually result in the ever increasing loads of dissolved solids found in the water. However, the changes in ion composition with increasing depth become more and more gradual with the exception of cases when highly soluble evaporite minerals such as gypsum or halite are encountered. Along the groundwater flow line, water from different sources is mixing as a result of dispersion and diffusion. Special attention needs to be focused on the very old brines that are found in the deepest parts of most sedimentary basins. It is believed that high loads of chloride salts were derived from solutions infiltrating from evaporating basins, ancient seas, the dissolution of salt deposits or fluids rising from the deeper crust or even mantle (e.g. Drever, 1997).

Precipitation and infiltration

The dissolved solids in precipitation are naturally derived from two major sources: seaborne salts delivering mostly chloride and sodium ions and terrestrial aerosols contributing mostly calcium and magnesium cations and bicarbonate as anions.

Infiltration water in humid climatic conditions, with the common presence of easy-to-weather carbonate minerals like calcite and dolomite, results in the predominance of HCO3-Ca-Mg water. The TDS of such water is usually around 0.2 to 0.5 g/l. In some cases the TDS value exceeds 0.7 g/l, bicarbonate might not be the dominant anion and chloride or sulphate can be present in a significant proportion.

Most of the Quaternary sediments contain calcite and dolomite. These minerals are the primary target of acid weathering in soils and the deeper part of the section. Calcium is leached much more readily than magnesium. However, the simulations with PHREEQC demonstrated that, thermodynamically, a system where water, carbon dioxide, calcite and dolomite are in equilibrium, the Mg^{2+} to Ca^{2+} molar ratio is approximately 0.7 and this is observed in field data as well. Significant Ca excess over Mg is observed rarely, mostly at a shallow depth. Kinetically calcite is less resistant to weathering and Ca-dominated waters may initially form. These are gradually transformed in Ca-Mg waters as the dolomite dissolution or even dedolomitization – dolomite dissolution and associated calcite precipitation – progresses. The highest bicarbonate concentrations are reached if the dissolution of carbonates takes place in an open system, that is, CO_2 is readily added from the atmosphere as the reaction progresses (Drever, 1997). That is in opposition to the dissolution taking place in a closed system – isolated from the atmospheric source of the CO_2.

This is the most significant process determining the composition of water found in the freshwater zone as a whole. There is no reason to believe that the weathering of alumosilicates plays any significant role in shaping the groundwater composition apart from the very top-most weathered soil layer where the carbonate minerals are outwashed. In most cases the dissolution of carbonate minerals present in most quaternary sediments will proceed much faster, neutralising the carbonic acid and organic acids derived from the soil and the atmosphere.

A very specific case of geologically recent groundwater recharge is known from Northern Estonia. Here the $\delta^{18}O$ value of the groundwater in the Cambrian – Vendian aquifer can be as low as -18 to -22‰ and the average modern precipitation values are from -8 to -11‰ VSMOW (Raidla et al., 2009; Vaikmäe et al., 2008). The TDS of this isotopically light water ranges between 0.2 and 1.3 g/l with a median around 0.5 g/l (Raidla et al., 2009). The low $\delta^{18}O$ value is explained by the intrusion of glacial meltwater in the aquifer. The relict water is trapped here due to the peculiarities of the geological structure – very low infiltration rates of the precipitation water through shielding local and regional aquicludes. The chemical composition of the groundwater changes from Cl-Na to HCO_3-Ca. The mixing of three end members – Cambrian brines, glacial meltwater and modern infiltration water – is used to explain these observations.

In Lithuania, the $\delta^{18}O$ value decreases as low as -13‰ (Mokrik et al., 2008). However below the depth of around 600 m increase of the $\delta^{18}O$ value is observed (Mokrik et al., 2008). This can be explained by the preservation of the remnants of glacial meltwater or precipitation water from cold stages in the deepest part of the active water exchange zone and the growing influence of deep-seated brines with $\delta^{18}O$ values as high as -5‰.

Ion exchange might have a role to play in controlling the cation contents in some particular cases. Cation exchange is an unsteady state process – it scraps the cations bound to the exchange sites on clay minerals. If the process operates for an infinite length of time with unchanged inflowing water composition, equilibrium will be eventually reached and water composition will not change any more. However, if the inflowing groundwater composition has changed significantly in geologically recent times, rocks will preserve a "memory" of earlier water composition in the form of cations bound to negatively charged sites on clay mineral surfaces (Sun et al., 2012; Ingebritsen et al., 2006).

In particular, HCO_3-Na type water reported from the Kaliningrad region in Cretaceous and Palaeogene sediments containing abundant glauconitic and Northern Estonia Cambrian and Vendian sediments (Jodkazis, 1989) are likely to be the product of ion exchange. Ca-rich bicarbonate water entering clay rich sediments can lose some of its Ca and extract some Na in ion-exchange reactions.

Oxidation – reduction systems

Significant concentrations (above 10 mg/l) of free oxygen are observed only at the very topmost part of groundwater that is in direct contact with the atmosphere (air in the pores of the sediments). Oxygen is consumed for the oxidation of organic matter abundant in groundwater and in most cases its concentration is below the limit for detection.

Oxidation of organic matter by O_2 consumption and other oxidisers such as nitrate ions and trivalent iron compounds results in CO_2 production in groundwater. Increased carbon dioxide concentration facilitates the weathering of carbonates or – if carbonates are not present – alumosilicate minerals – resulting in the formation of bicarbonate water with various proportions of cations.

Bacterial sulphate reduction and the formation of H_2S bearing water is noted on a few occasions: Ķemeri and Baldone in Latvia and Lieknu near Biržai in Lithuania. The H_2S concentration can reach 70 mg/l, however, it is highly variable (Jodkazis, 1989). An examination of the largest H_2S water field near Ķemeri (Prols, 2010) suggested that the presence of any organic compounds in the water does not necessarily mean that bacterial reduction of inorganic compounds that are present will take place. However the reducing capabilities of an organic rich solution can be boosted by an admixture of oxygen rich water that can trigger partial oxidation of organic matter and the production of simple organic compounds, suitable for consumption by sulphate reducing bacteria.

Often increased dissolved iron and manganese concentrations are observed (Hiiob and Karro, 2012). In most cases (>90%) the load of dissolved iron is less than 2 mg/l, however, occasionally it can exceed 10 mg/l. Higher dissolved Fe values usually are associated with terrigenous rocks (Levins and Gosk, 2008), however, this is not a universal observation. In the terrigenous D_3 Gauja aquifer the usual ferrous iron (Fe^{2+}) load is 0.5 mg/l, while in the dolomite D_3 Pļaviņu aquifer a concentration of around 0.25 mg/l is most often observed. The manganese concentration rarely exceeds 0.2 mg/l and in most cases is less than 0.03 mg/l. The reduced, bivalent forms of both iron and manganese are mobile in waters with neutral or slightly alkaline pH values. In contact with atmospheric oxygen, both elements are readily oxidised and precipitated as $Fe(OH)_3$ and MnO_2 respectively. The observed concentration of iron is poorly correlated with other parameters and its regional distribution is not well understood.

Dissolution of evaporite minerals

The occasional presence of gypsum bearing sediments results in the formation of SO_4-Ca type water (reaction 1). However, as noted by Jodkazis (Jodkazis, 1989) in contrast to many other artesian basins, a distinct zone of sulphate waters is missing within the BAB. Gypsum dissolution is often accompanied by a dedolomitization reaction that consumes dolomite and calcium ions and produces calcite, and releases magnesium ions into the solution (reaction 2). Dolomite is usually present in sedimentary rocks alongside gypsum. As a result, a rather constant magnesium to calcium ratio is observed. The dissolution of gypsum is a fast process while the dedolomitization takes a while and so calcium-dominated as well as calcium-magnesium type sulphate waters can be encountered. An increase in Ca concentration induces the precipitation of calcite (reaction 3) forcing down the bicarbonate concentration (Figure 1.).

As accessory mineral gypsum is found in the Narva formation and underlying Lower Devonian sediments, particularly in the Eastern part of the basin (Misāns, 1979), as a result sulphate-type waters are found below it in the Middle-Lower Devonian aquifers.

Gypsum deposits in Upper Devonian carbonate formations as well as those associated with Permian evaporite sediments are well known. The south-western part of Latvia and the north-eastern part of Lithuania are regions where sulphate-type waters are widespread in the mostly carbonatic sediments of the upper part of the Frana stage and the Upper Devonian. The resultant sulphate water body extends from the Kursa uplands into the western part of the Zemgale lowland into the D_3 terrigenous Gauja and Amata aquifers.

In the south–western part of Lithuania and in the Kaliningrad region, a salt bearing Prieglius (*Преголъской*) formation of Permian age is found. The bottom part of the formation is mostly composed of anhydrite while halite and potassium salt make up the upper part (Jodkazis, 1989). Brines originating from the dissolution of Permian evaporites (salt) are found in the upper part of the sedimentary cover in the south-west part of the basin, where TDS values in the aquifers above and below salt-bearing formations range from 34 to 304 g/l. Below dissolution brines water with a smaller TDS can be found – e.g. density inversion is reported. These waters are characterised by a particularly low value of dissolved Br – not more than 292 mg/l even for the strongest brines.

In the valleys of the Nemunas River and its tributaries, saltwater originating from evaporite dissolution is seeping upwards, mixing with freshwater and in places reaching the earth’s surface.

At the base of the Narva formation, Middle Devonian pseudomorphs of halite crystals are reported (Misāns, 1979). So, the presence of halite itself in this aquitard

$$CaSO_4 * 2H_2O \rightarrow Ca^{2+} + SO_4^{2-} + 2H_2O \quad (1)$$

$$Ca^{2+} + (Ca,Mg)CO_3 \rightarrow CaCO_3 + Mg^{2+} \quad (2)$$

$$Ca^{2+} + 2HCO_3^- \rightarrow CaCO_3 + H_2O + CO_2 \quad (3)$$

A

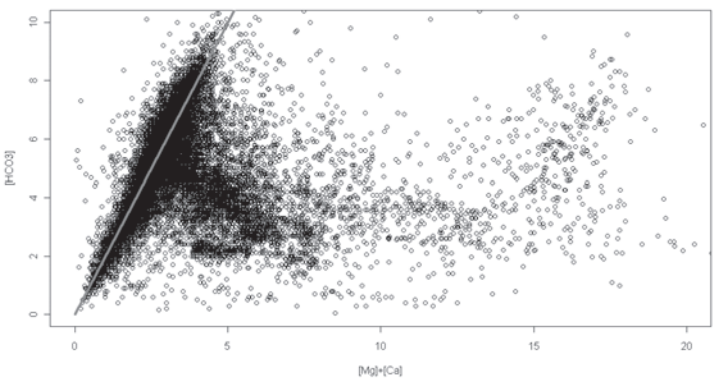
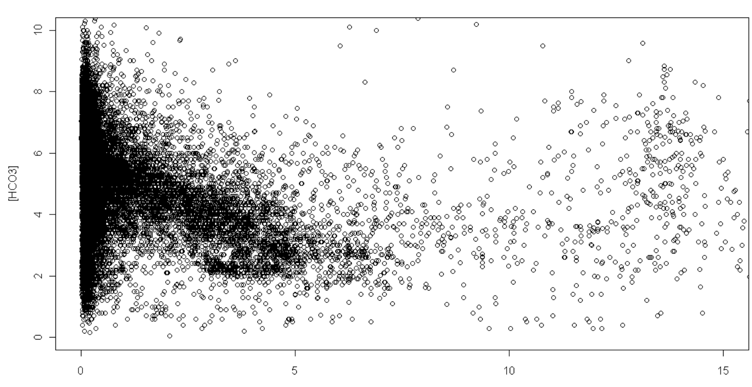


Figure 1. The relationship of the molar concentrations of HCO3- and Ca^{2+} and Mg^{2+} ions (A), where the grey line in the image indicates the equiv.-molar relationship, and SO_4^{2-} ion HCO_3^- ion

B



(B) in the groundwater above Narva aquiclude in Latvia.
The decrease of the bicarbonate concentration in association with an increasing sulphate concentration indicates calcite precipitation associated with gypsum dissolution.

cannot be ruled out completely and it could be the source of elevated salinity in the underlying D_{1-2} aquifer. Raidla (Raidla, 2010) discussed that the observed water composition including stable isotope data in north-eastern Estonia can be explained by salt dissolution.

Formation brines

Huge reserves of Cl-Na-Ca or Cl-Ca-Na formation brines (that is very salty water usually found at great depth) reside in the deepest part of the Baltic Artesian Basin. In most parts of the basin in the deepest aquifers, the TDS commonly is above 100 g/l and can exceed 180 g/l. On the basis of macro-components two water types can be distinguished: the Cl-Na type and the Cl-Na-Ca type (Figure 2.). The increase in mineralization is accompanied by an increase in the chloride normalised Na/Ca value: the relative Na component of all cations is diminishing and Ca – increasing. Ca-rich brine is found in the deepest – South-Western part of the aquifer. It is noted that the concentrations of minor components is different as well, e.g. the Cl to Br ratio is around 260 at the Latvian saddle and 155 at the Baltic syncline. The content of dissolved gases contrasts as well: in the Latvian saddle N_2 is dominant, while in the Baltic syncline the content of hydrocarbons increases with depth and so does argon free nitrogen gas – biogenic N_2. Similarly, CO_2 concentration is higher in the western part of the territory (Levins, 1990).

Dilution of the formation brines with freshwater is observed in the shallow part of the basin. For example in northern Estonia in the Ordovician – Cambrian aquifer and Cambrian – Vendian aquifer, HCO_3 dominated freshwater (TDS 0.2 to 1.8 g/l) is found (Raidla et al., 2009). Complex water composition evolution is suggested by the rather contrasting chemical composition mostly illustrated by the transition from Ca-HCO_3 to Na-Cl types, but in-between includes peculiar Na-HCO_3-Cl type water with a sodium bicarbonate proportion, increasing in the waters with TDS from 0.4 to 1.0 g/l (Jodkazis, 1989). However, freshwater is readily replaced by mostly Na-Cl brines in southern Estonia where TDS reaches 22 g/l and already above 100 g/l in northern Latvia.

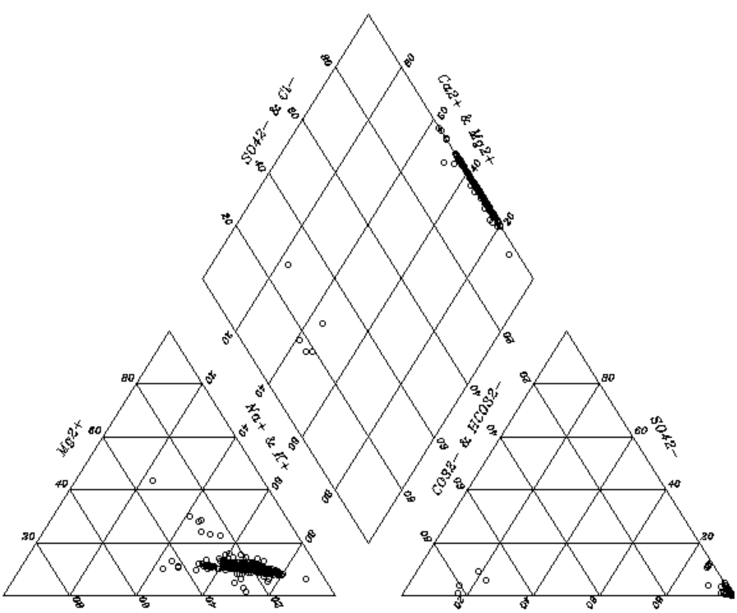


Figure 2. The groundwater composition in the Cambrian aquifer and Ordovician – Silurian aquiclude in Latvia.

Density inversion is reported in some cases: denser, more saline brine is found above less dense brine sampled in the same boreholes (Jodkazis, 1989). This could be the result of the geologically recent intrusion of subglacial meltwater associated with preferential pathways with higher conductivity.

Hydrocarbons – oil and natural gas – are found in the deepest, southern and western part of the Ordovician – Cambrian aquifer (Jodkazis, 1989). Most notably the occurrence of considerable stocks of hydrocarbons is associated with the particular composition of the dissolved gases: increased concentrations of CO_2 and up to 40% of molecular biogenic nitrogen, marked by a low content of inert gases. In the rest of the territory, nitrogen makes up 75 to 98% of all dissolved gases, while hydrocarbons are less than 1% and inert gases 0.9 to 2.3%.

A gradual shift from Cl-Na to Cl-Ca-Na type brines is observed moving from more shallow to deeper parts of the basin. It is likely that the process of albitization (Davisson and Criss, 1996) is responsible for this trend. It is suggested that in most of the world's sedimentary basins albite (Na-feldspar) formation and plagioclase (Ca-Na feldspars) dissolution is responsible for the increased Ca-ion concentration in the brines relative to sea water. Albitization proceeds faster with increasing temperatures that usually strongly correlate with the depth of the aquifer. Coincidentally, the brine strength increases with depth as well. In the brines with a TDS above 125-130 g/l Na is largely substituted by Ca, and proportion of Na equivalents can be less than 45% of all cation-equivalents. Temperature rather than brine concentration could control Na removal and Ca enrichment.

The observed Cl^-, Na^+ and Ca^{2+} concentrations fit nicely on the basin fluid line introduced by Davisson and Criss (1996): Na deficit and Ca excess compared to modern seawater (Figure 3).

The decrease in sulphate ion concentration in the SW (Baltic syncline) noted by Levins is likely due to the increased Ca^{2+} concentration that is replacing Na^+ and as a result the equilibrium is shifted toward precipitation of calcium sulphate. This is supported by the simulations with PHEERQC.

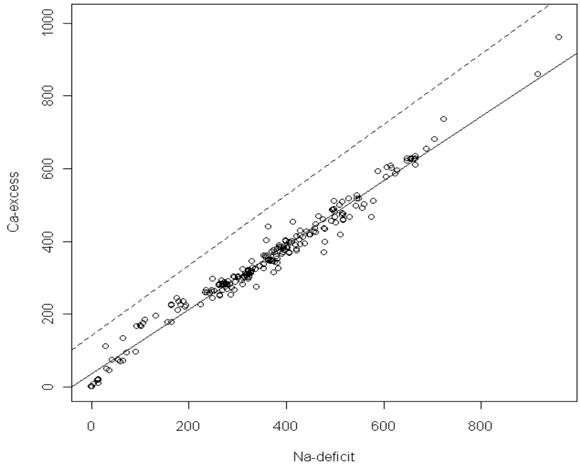


Figure 3. Na-deficit / Ca-excess expressed in the mmol-equivalent/l indicating the extent of the sodium replacement with calcium ions in the brine in respect to sea water. Solid line – calculated regression for the observations in Latvia; dashed line – global basin fluid regression line (Davisson and Criss, 1996).

Interestingly, a particularly low Na^+ concentration is observed in the crystalline basement in north-western Estonia. Here the Ca^{2+} concentration measured in eq/l can exceed Na^+ concentration by up to two times (Karro et al., 2004), while the TDS is only 2-22 g/l (Raukas and Teedumäe, 1997). Such a low Na^+ content in respect to Cl^- is not observed even in the deepest parts of the basin in Latvia and Lithuania. Perhaps it is too simplistic to postulate that such water composition originates from seawater as a result of extensive albitization and some dilution with freshwater – a more complex history is likely.

Mantle degassing and metamorphic waters can contribute to groundwater composition, particularly with respect to the brines found in deep stagnant aquifers (e.g. Pinti et al., 2011). Research in Estonia has demonstrated that enrichment of water with certain micro-components, particularly barium, can be explained by groundwater interaction with the weathered crust of the crystalline basement (Karro et al., 2009)

There is evidence that, at least locally, upward leakage of deep saline groundwater – salt water intrusion into the predominantly freshwater zone – is taking place. It can be seen particularly well in places where saline water from a greater depth is infiltrating the aquifers exploited for water supply, like the terrigeonus aquifer complex of the Middle-Upper Devonian in Latvia. In such places large well densities allow good identification and characterisation of chemical anomalies.

A region of increased groundwater salinity is found in the south east part of the basin in the vicinity of Druskinaiki, Birštonas and Stakliškės (Jodkazis, 1989). In the Quaternary sediments, the TDS can rise up to 1.5-3.0 g/l and reach 57 g/l at the bottom part of the Triassic aquifer (Jodkazis, 1989). Here even saltwater springs are found in the river valleys. It is suggested that this region was a discharge zone for the deepest aquifers when most of the BAB was covered by Pleistocene glaciations and groundwater flow was reversed (Zuzevičius, 2010). Upwards seepage of saltwater is observed in other places as well, especially where deep river valleys coincide with tectonic fault lines.

There is a prominent body of salt rich water below the City of Riga. Its northernmost part is already traceable near Carnikava. In the S direction, it splits into three parts, with two confined to the deepest part of the aquifer, both to the E (Ulbroka and Saurieši vicinity) and to the W (Piņķi, Babīte and Skulte vicinity) of the City of Riga, and a third confined to the top of the aquifer, close to the centre of the city. Further to the south only moderately low chloride concentrations are observed. It is suggested (Levins, 1990) that there is water seeping upwards from below Narva formation, as this region coincides with the channels of all the major rivers and thus is the regional groundwater discharge area. This is supported by the results of hydrogeological modelling showing upward groundwater flow across the regional Narva aquitard.

Intensive water abstraction in the Kopli Peninsula, Tallinn, has led to up flow of saline water from the crystalline basement (Karro et al., 2004) as well compromising the water quality.

Anthropogenic influences

A number of anthropogenic activities such as intensive agriculture and water abstraction, including for the drainage of the mines and quarries, and environmental pollution are influencing groundwater composition.

Apart from the point sources of the pollution, two major processes of agricultural influence on groundwater composition can be identified: the inflow of pollutants such as fertilizers and the remains of pesticides and the activation of weathering processes due to the ploughing of soil and the establishment of drainage systems (Levins and Gosk, 2008). Environmentally, the most important are pollution with nitrogen compounds (nitrate ion and ammonium) and phosphorus derived from fertilizers. These compounds can cause the eutrophication of surface water bodies where groundwater is discharging. However, increased loads of chlorine and a range of micro-components such as uranium, rubidium and many other are derived from the fertilisers as well. The decrease in groundwater level as an irrigation measure intensifies the infiltration of precipitation water and the ploughing of soil exposes fresh mineral surfaces to weathering. As a result the leaching of bicarbonate and major cations from agricultural lands is increasing.

Groundwater composition certainly has changed within urban areas. For example, an increasing trend of sodium and chlorine ion concentrations has been observed in Riga at a single groundwater monitoring station (Raga et al., 2012). This can be best explained by the flushing of the salt applied on streets during winter into the aquifer below.

The composition of groundwater is certainly affected by the changing composition of precipitation water (Treier et al., 2004). In the case of major ions, the increased loads of sulphur, chlorine, calcium and magnesium originate from the use of fossil fuels like oil-shale and the aerosols associated with the cement industry. However, the magnitude of these sources and the buffering capacity of the environment remain poorly quantified.

Intensive oxidation of pyrite is taking place in the region influenced by the depression of the groundwater level around oil-shale mines in north-eastern Estonia. Oxygen rich infiltration water is percolating down to the lowered water table around the oil-shale mines oxidising the pyrite found in mostly carbonate cover rocks. The resultant sulphuric acid is immediately neutralised by the carbonates and SO_4-Ca water is produced (Erg, 2005). The direct oxidation of pyrite by oxygen (reaction 4) in the extended aeration zone or pyrite oxidation by Fe (III) compounds (reaction 5) are the likely mechanisms for sulphate production (Erg, 2005).

$$FeS_2 + \frac{15}{4}O_2 + \frac{7}{2}H_2O \rightarrow Fe(OH)_3 + 2H_2SO_4 \qquad (4)$$

$$\begin{aligned} &FeS_2 + 14Fe^{3+} + 8H_2O \rightarrow 15Fe^{2+} + 2SO_4^{2-} + 16H^+ \\ &Fe^{2+} + \frac{1}{4}O_2 + H^+ \rightarrow Fe^{3+} + \frac{1}{2}H_2O \end{aligned} \qquad (5)$$

Intensive water abstraction in the costal cities can result in the infiltration of sea water to groundwater. In a few costal cities like Liepaja, Tallinn, Parnu, Haapsalu and Kingisep extensive sea water intrusion due to overexploitation of groundwater can be observed (Jodkazis, 1989). However, natural storm surges (wind-driven local sea level rise) and windblown sea water droplets can increase the salt content of groundwater in coastal settings up to 0.8-1.7 or even 5-6 g/l (Jodkazis, 1989). One of the best known examples is in the city of Liepāja, where the mixing of sea water and fresh bicarbonate groundwater can be observed (Figure 4). Seawater intrusion is taking place in the Upper Devonian Mūru-Žagari aquifer. A Na exchange for Ca ions as seawater enters previously freshwater bearing aquifers can be inferred.

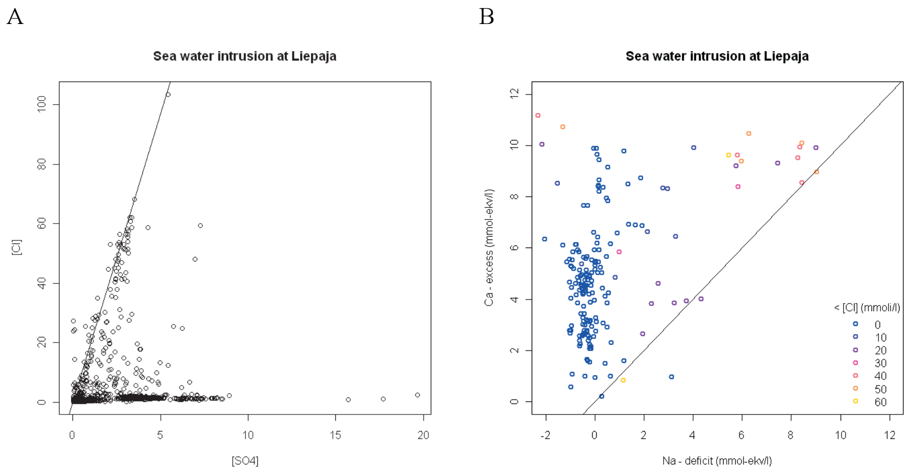


Figure 4. Illustration of groundwater composition within Liepāja city, in the multiple aquifers above the Narva regional aquiclude: A – the chloride and sulphate concentration (mmol/l), the line indicates simple mixing between seawater and fresh water; B – Na-deficit / Ca-excess graph (Davisson and Criss, 1996), the line indicates the simple substitution of the Na by Ca ions in diluted seawater – bicarbonate freshwater is naturally enriched with calcium ions, high salinity waters (pinkish to yellowish dots) show some enrichment with calcium at the expense of sodium. It can be speculated that this is due to ion exchange with the sediments.

Concluding remarks

The presence of major regional aquitards in the basin delineates the geochemical water zones as well as water exchange zones. As the basin grows deeper from north to south, so newer sedimentary rocks can be found below the Quaternary sediments and the number of aquicludes increases. In northern Estonia, freshwater is present in the full thickness of sedimentary rocks. In the direction to the south the Silurian-Ordovician sediments grow thicker and gradually turn from a carbonatic aquifer to a major regional aquiclude comprising schist, marls and dolostones (Misāns, 1979). In association with this, the salinity of the water in underlying Cambrian-Vendian sandstones gradually increases from freshwater in northern-Estonia to brines in northern Latvia.

Of the Lower Devonian – appears in south Estonia. It is composed of dolomitic marls, carbonatic clays, siltstones and dolomites and gypsum as the usual secondary mineral. At the base of the formation, even pseudomorphs of halite crystals are reported (Misāns, 1979). Meanwhile in Estonia, freshwater is found in the Lower-Middle Devonian sandstone aquifer below the Narva formation; already in the northern part of Latvia, salinity gradually increases reaching over 30 g/l in the south-eastern corner of Latvia. The zone of waters with intermediate salinity is traditionally termed the stagnant water exchange zone, indicating that slow mixing of infiltration water and relict brines is taking place here, allowing plenty of time to progress the interaction between the water and the rocks.

A good example of the nature of chemical zoning is the Lower-Middle Devonian aquifer (Figure 5). The HCO_3-Ca-Mg freshwater with a TDS ranging from 0.5 to 0.6 g/l occurs in the Middle-Lower-Devonian aquifer system in southern Estonia (Raukas and Teedumäe, 1997) and northern Latvia. As the aquifer deepens mostly chloride type salt water replaces freshwater and salinity can reach 33 g/l in the central part of the Latvian saddle and 117 g/l in the deepest part of the Baltic syncline in the SW of the basin (Jodkazis, 1989). Sulphate water with moderate mineralization is fond in the SE part of the basin where the aquifer is shallow and gypsum is found both in the confining Narva formation and the middle-lower Devonian terrigenous aquifer itself (Jodkazis, 1989). Distinct chemical zoning can be observed even within the aquifer itself in the SW part of Latvia: the chloride concentrations are markedly higher in the deeper part of the aquifer complex, that is Lower Devonian sediments compared to the upper part of the aquifer (Middle Devonian sediments), while sulphate content remains moderately high in both parts of the aquifer.

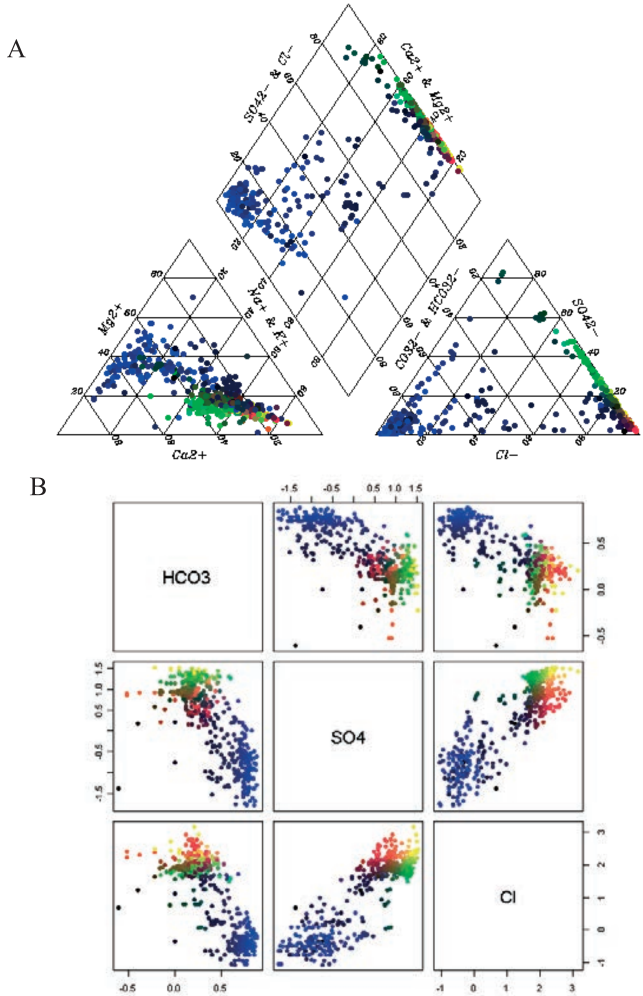


Figure 5. Water composition in the D12 aquifer: A – piper plot; B – scatter plot for scale, concentrations in *log(mmol/l)*. Red is proxy for chloride, green for sulphate and blue – for bicarbonate anion. The blue points are bicarbonate dominated freshwater found in the Northern part of the aquifer, while the green points represent the sulphate water of the upper part of the aquifer in the Baltic syncline and the red points represent the chloride dominated water at the base of the aquifer in the Baltic syncline.

Groundwater origin and evolution is a complex question and even the definition of the question can be ambiguous because very often migration occurs and the speed of water molecules and different dissolved species don't follow the same rules. No doubt there is a geological record hidden in the composition of groundwater, however, its description is not straight forward.

Acknowledgements

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Groundwater abstraction in the Baltic Artesian Basin

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Abstract

Groundwater abstraction for the domestic and industrial water supply in the Baltic countries has been analyzed. Due to the varying quality of data sources, different data interpolation and extrapolation methods have been applied to fill the gaps in the data set on groundwater abstraction in the Baltic countries for the period 1900-2010. The general trends in groundwater use have been found and three main scenarios based on the groundwater abstraction rate are outlined: the natural scenario, the wasteful scenario and the sustainable scenario. Groundwater modelling using the MOSYS hydrogeological model system was applied for the simulation of long-term effects of different groundwater abstraction scenarios. Current groundwater abstraction amounts have been proved to be sustainable for long-term use of groundwater.

Keywords: groundwater amount, depression cone, water abstraction scenarios

Introduction

Groundwater has been the source of the domestic and industrial water supply in the Baltic countries for more than one century, but more intensive groundwater abstraction commenced in the middle of the 20th century. Today centralized as well as decentralized water supply mainly depends on groundwater resources. Groundwater abstraction has changed the natural hydrogeological conditions in the Baltic Artesian Basin (BAB). Therefore, it is necessary to define the amount of groundwater already extracted as well as the amount of prospective resources in order to develop a responsible, environmentally friendly and sustainable water abstraction regime for the area of the Baltic Artesian Basin. In order to find the best water supply scenario, the most essential part is data collection and analysis, followed by the modeling of piezometric head distribution based on the variable water abstraction data.

Data sources

The availability and quality of data on groundwater abstraction varies in time and space. Different data sources which complement each other are used in order to obtain a complete water abstraction data set which covers the territory of the Baltic countries since reasonable groundwater abstraction began, i.e. the beginning of the 20th century. The compilation of a complete data set was done in several steps: 1) gathering of all recorded data on groundwater abstraction; 2) data analysis and verification; 3) filling of gaps in the recorded data by applying data interpolation and extrapolation.

The water abstraction data in Estonia was obtained from the data base on available resources of about 2000 boreholes maintained by the Geological Survey of Estonia. Within the frame of the BAB modeling system (MOSYS), this data set covering very detailed information of the tiniest boreholes is the most complete of all of the available information provided by other sources and provides a very good description of the historical situation of water extraction in the 20th century as well as nowadays.

The water abstraction data in Lithuania is based on the recorded data in 2009 from each of the water extraction sources, where water abstraction is above 100 m^3/day, and was provided by the Geological Survey of Lithuania. The change in water abstraction over time was based on the published data on total groundwater use in 1945-2000 (Juodkazis and Klimas, 2003). The general trends of groundwater abstraction were analyzed and then applied to the existing data set from 2009. Although this approach cannot yield a reliable data set for the detailed analysis of groundwater use in Lithuania, a rough estimation was achieved for running the transient state calculations of the BAB modeling system.

The data on groundwater abstraction in Latvia for the BAB modeling system was gathered from many data sources due to the lack of one complete historical data set. Most of the available information refers to the 244 wellfields and groups of wells in Latvia without any detailed information about the separate wells forming the corresponding sources of water. The main data sources giving true information were: for 1975 – 1993, copies of water abstraction reports held in the Latvian Geological Fund (e.g. Levina and Dumpe, 1980; Tolstovs and Levina, 1976; Tolstovs et al., 1986 etc.); for 1998 – 2007, information gathered by the Latvian Environment, Geology and Meteorology Agency (LEGMA) and published in the reports on groundwater balance (e.g. Levina and Levins, 1994) and for 2008 – 2010, water abstraction data was collected from the reports on groundwater balance prepared by the the Latvian Environment, Geology and Meteorology Centre (LEGMC) and published on the web (e.g. LVĢMC, 2009). Some estimations were used to add the available true data set: the estimations used in the regional hydrogeological model program REMO (Spalvins et al., 1996) giving the data on summarized water abstraction from the 34 largest water extraction sources and the expected percentage of water abstraction from each aquifer used for the corresponding source of water; the estimations for 1980 were based on the known change of total water abstraction as well as the industrial water consumption rate in the largest cities, comparing the 1980 to 2008. In addition, any kind of information was used that helps to reconstruct water extraction within the actual time interval 1900 – 2010, for instance the information about the installation year of the groundwater sources and if the source of water was closed – the closing year. An assumption was made that before the installation of the first borehole in any of the water extraction sources, groundwater consumption was impossible, and that it was impossible after the closing of the water source. Therefore, the water extraction amount was considered as 0 cubic meters per day in these cases.

Although many data sources are used to obtain a water extraction data set for the BAB model in Latvia, there are many empty gaps in the actual years 1900 – 2010, especially from the years 1994 – 1998. As any kind of water abstraction data from groundwater extraction sources was collected and not from single wells, one can make the statement that after the installation of each water extraction source, water was consumed every year, especially if the source of water refers to the centralized water supply of a city or town and these previously mentioned empty gaps should be filled with reasonable numbers, and therefore, data interpolation and extrapolation was applied. To keep the extrapolated and interpolated numbers reasonable, the information on total groundwater abstraction in 1960 – 1998 provided by Levins et al. (1998) and in 1996 – 2004 provided by the LEGMC was used (Figure 1). To perform mathematical processing of the gathered data, various types of extrapolation and interpolation methods were used there: exponential extrapolation was used for older water extraction sources (older than 1960); logarithmic extrapolation was usually used for newer water extraction sources (newer than 1960); in some special cases linear extrapolation was used; linear interpolation was usually used for a year which was lacking data; second or third order polynomial interpolation was used to fill the empty gaps between 1990 – 1997, where the previous and next 5 years of the actual empty gap period were taken into account to perform a better match with the real data.

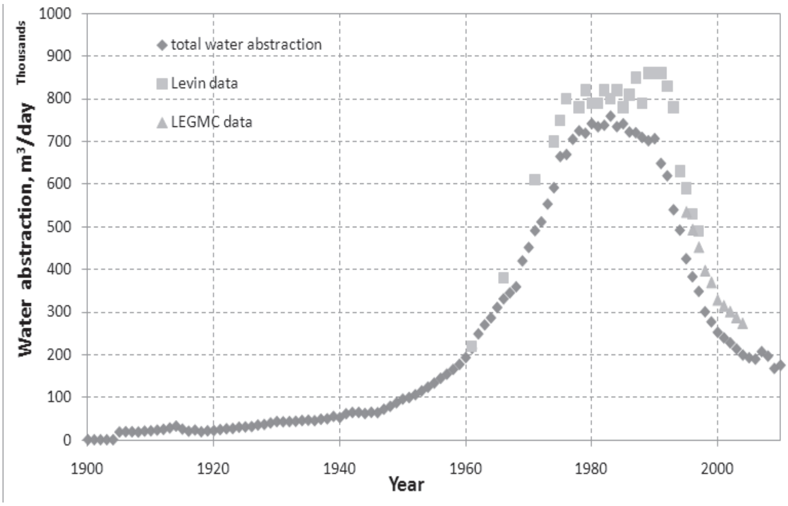


Figure 1. Groundwater abstraction in Latvia in 1900-2010, thousands m^3/day. Data from references on total water abstraction (darker dots) and the result of extrapolation and interpolation (lighter dots).

A snapshot of the resulting data set is shown in Figure 2 – the table consists of 244 rows depicting water extraction sources where the columns are the years, starting from the left with the year 1900 and ending on the right with the year 2010. The column for 1980 is surrounded by a dark black line, while the column of 2009 – by a thin black line. The large amount of orange colour shows how many empty gaps have been filled by interpolation or extrapolation methods. One can especially see that there is very little recorded data in 1990 – 1997, which corresponds to a very poor match between the published and interpolated data shown in the graph in Figure 1. The light yellow colour shows the added data on such essential information as the depth of a filter or the installation date of very new water extraction sources, which were installed mostly after 2000. The information on the depth of filter for multi-aquifer systems was found using the BAB model, according to the reference information about the used aquifer and the location of the water source; the dates of installation of very new water sources were found in published documents of summaries of the corresponding water extraction source. The green colour shows the data which was gained by estimation. Although the estimated data sources are added to the true data set, usually the years of the given estimated data cover the true data set (in white color) or are completely incompatible with the true data set; therefore, the use of estimated data is very limited without any additional information on how the estimations in the other studies were made. The water abstraction data in Latvia for the BAB modeling system was based mainly on true data and data extrapolation and interpolation.

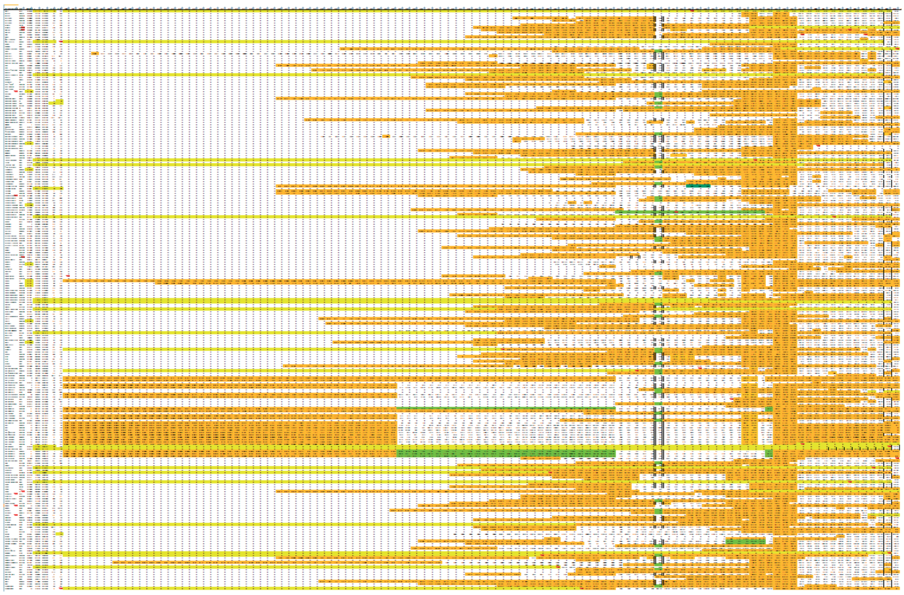


Figure 2. The snapshot of water abstraction data set in Latvia; light yellow – added data from different information sources; orange – interpolated or extrapolated data; green – estimated data; white – true data.

In Figure 1, one can see that there are slight differences between the published data and gathered data for the BAB modeling system, especially in the period 1970-1990, where our estimation is lacking about 50 thousands m^3/day of water extraction in Latvia when referring to the published data. There are several reasons for that: 1) the data sources in Latvia gave very fragmentary data and estimations and mathematical methods have to be used to fulfill the data table from 1900 to 2010 (Figure 2); 2) water abstraction in cities, towns and the largest settlements were taken into account in our estimation: single water sources in rural areas with water abstraction less than 100 m^3/day were not included in this data set. In addition, one should take into account that the mathematical processing tends to perform smoothing between the known data; therefore if there must be any rapid changes (like there may be during 1990 – 1997), they will remain unknown and cannot be predicted precisely without any true or estimated data.

Groundwater abstraction - amounts and sources

Total amount of extracted groundwater

When data collection and processing is done, the result is a table containing all the information about every available record – the water extraction source ID number, the name of the aquifer, the x and y coordinates, the depth of the filter and the amount of abstracted water in 1900 – 2010. This data set gives us a possibility of making a data analysis, beginning with the total amount of abstracted water in Latvia, Lithuania and Estonia (Figure 3).

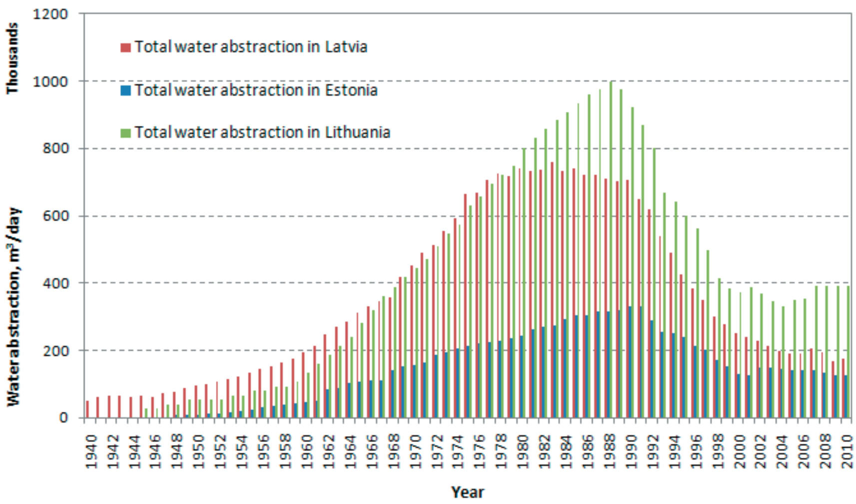


Figure 3. Total groundwater abstraction in the Baltic countries.

The rapid changes in groundwater abstraction are shown by the data. Until 1950, groundwater abstraction had been insignificant in the Baltic countries, but in the period 1950 – 1990, a rapid increase in groundwater abstraction occurred, especially in Latvia and Lithuania. This rapid increase in groundwater extraction was due to the growth of industrial and rural activities, the installation of a great number of wells in rural areas and the establishment of wellfields for the centralized water supply systems for towns and cities.

After 1990, there was a sizable reduction that lasted until the year 2000 when the total amount of water abstraction had become more or less stationary without any rapid increases or decreases. When comparing water abstraction in the years 1990 and 2010, one can see that the decrease in the amount of total water abstraction in Latvia was by about 4, in Estonia – by about 3, and in Lithuania – about 2..5. Besides, nowadays (2009-2010) the total amount of abstracted water in m^3/day in Latvia is only 50 thousand m^3/day more than in Estonia and 140 thousand m^3/day less than in Lithuania, whereas in 1990 the difference in total water abstraction between these countries was larger: in Latvia groundwater abstraction was about 375 thousand m^3/day more than in Estonia and about 200 thousand m^3/day less than in Lithuania. These changes may be explained by the sudden collapse of industry after the restoration of the independence of the Baltic countries.

There is one more aspect that shouldn't be left unnoticed – the different patterns in the total water abstraction graphs: in the period 1950 – 1990 in Estonia and Lithuania an even increase had been observed in total water abstraction, whereas in Latvia in the same period, the even increase lasted only until 1975, but after that there was practically a stationary plateau until 1990 without any further significant increase. Looking at the map of locations of water extraction sources in the year 1980 (Figure 4), which is about the middle of the interval between 1975 - 1990, the main trend of water source location was obvious – more water was usually abstracted near the largest cities: 1) in Latvia: Rīga, Jūrmala, Valmiera, Liepāja, Daugavpils; 2) in Estonia: Tallinn, Kohtla-Järve, Tartu, Rakvere, Viljandi etc. ; 3) in Lithiania: Vilnius, Kaunas, Klaipeda, Siauliai etc. The groundwater in these cities was mostly used for the centralized water supply and industry.

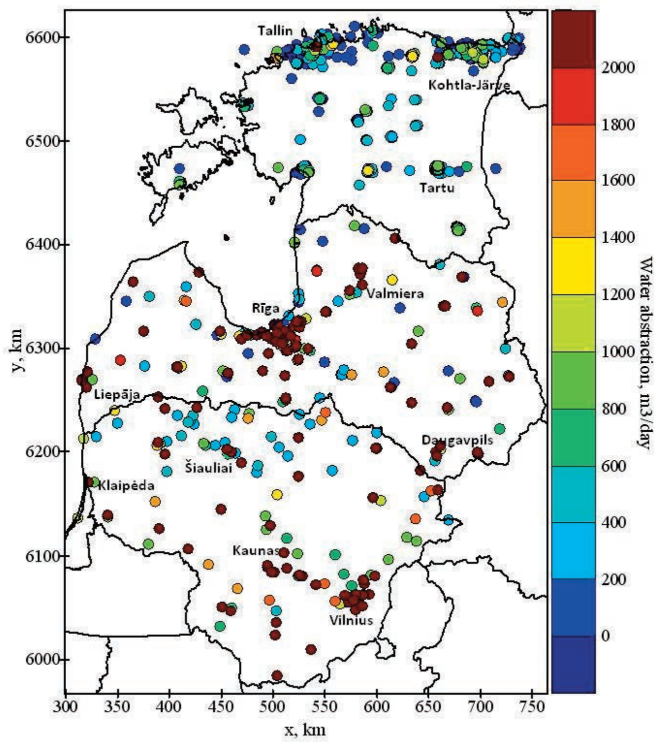
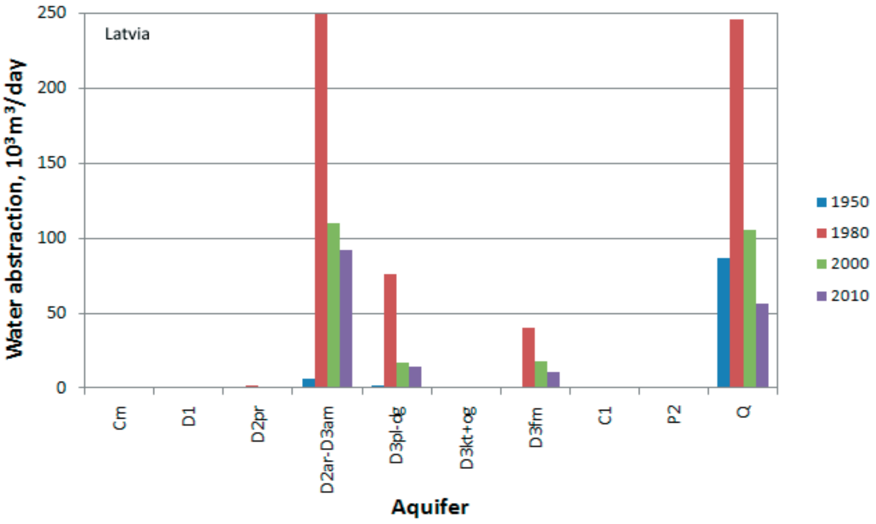


Figure 4. Map of groundwater extraction sources and amounts in the year 1980.

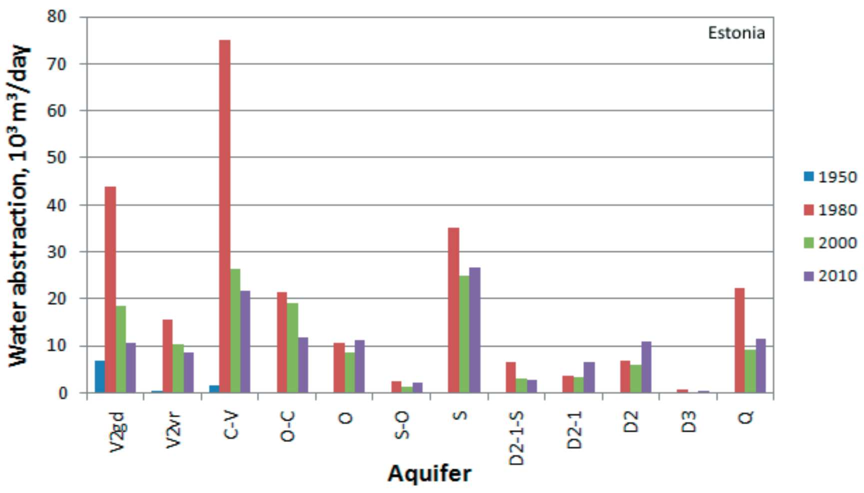
The explanation for the observed plateau in the period 1975 – 1990 for total water abstraction in Latvia was mainly due to changes in the drinking water supply in Riga. The concentrated intense groundwater abstraction in Riga city and its surroundings caused a significant decrease in groundwater levels in the middle Devonian Gauja – Amata aquifer and the formation of the so called "Large Riga" depression cone (Levins et al., 1998). Therefore, water abstraction from groundwater resources was limited and a likely stabilization in groundwater abstraction occurred. The need for a drinking water supply was met by increasing the water supply from surface water sources, like the River Daugava for the Riga and Daugavpils water supply, and Puze Lake for the Ventspils water supply.

Amount of abstracted groundwater by main aquifers and multi-aquifers

To gain a complete understanding about water abstraction in the Baltic countries, an analysis of total water abstraction is not enough. The water abstraction from each aquifer of the BAB must also be analyzed. This may provide information about the aquifers most vulnerable to overexploitation as well as the aquifers containing potential water resources. Four years were chosen to characterize the distribution of abstracted groundwater by aquifers: 1950 as the reference year when significant groundwater abstraction began, 1980 – the year, when groundwater abstraction was the most intense, 2000 – the time of a serious decrease in the abstracted water amount, 2010 – representing current groundwater abstraction. Figure 5 shows the aquifers used for fresh water abstraction and the amount of groundwater pumped in each country. In many cases in particular areas groundwater is simultaneously pumped from several adjacent aquifers, and therefore Figure 5 shows the main aquifers and multi-aquifers used for water supply.



a)



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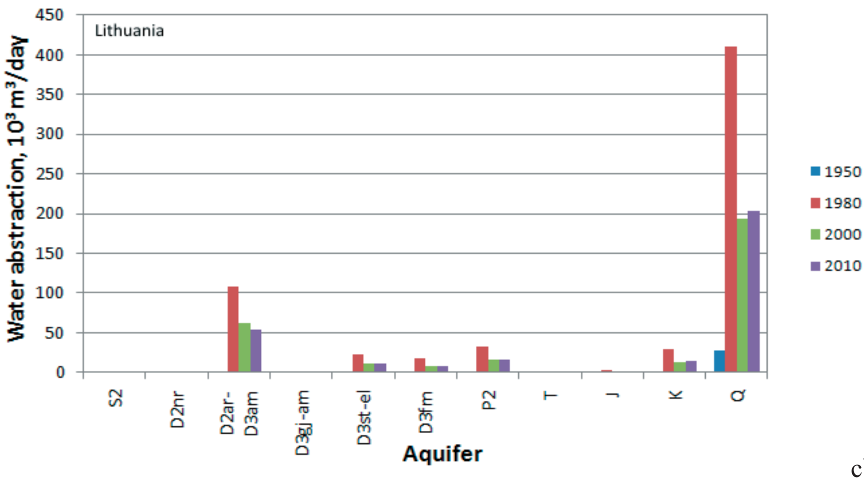


c)

Figure 5. Aquifers used as sources of fresh groundwater and the amount of abstracted water in representative years. a) Water abstraction from aquifers in Latvia, b) Water abstraction from aquifers in Estonia, c) Water abstraction from aquifers in Lithuania. Year 1950 - blue, year 1980 red, year 2000 green, year 2010 purple.

In Latvia, nowadays (considering this to be 2010) the most loaded is the middle Devonian Arukila – upper Devonian Amata multi aquifer (D_2ar-D_3am) with a total amount of 92 thousands m^3/day of abstracted groundwater. In this multi aquifer system, the most important is the upper Devonian Gauja (D3gj) and the Gauja – Amata (D3gj-am) aquifers with 22 thousands m^3/day and 35 thousands m^3/day of abstracted water respectively. This multi-aquifer is widely used throughout Latvia, except the eastern part, where the upper Devonian Plavinas – Daugava multi aquifer (D3pl-dg) is mainly used instead and about 15 thousands m^3/day of water are abstracted. The second most loaded is the Quaternary aquifer with a total amount of 56 thousands m^3/day. The highest consumption belongs to the centralized water supply of Rīga city (42,000 m^3/day) accounting for 75% of total Quaternary water abstraction, the second biggest consumer is Daugavpils city (13 000 m^3/day), which together with Rīga forms 98% of the total water abstraction from the Quaternary aquifer.

A significantly smaller amount of water is abstracted from the upper Devonian Famenian (D3fm) multi aquifer – only 10 thousands m^3/day, and mainly belongs to the water supply of Liepāja city and the nearby towns like Grobiņa and Aizpute. Water extraction from the deeper aquifers, the Cambrian (Cm), the lower Devonian (D1), and the middle Devonian Pērnava (D2pr) are insignificant –these aquifers contain mainly brackish and saline waters and brines in the Cambrian and it is mostly used for balneological purposes. The Middle Devonian and lower Devonian aquifers in northern Latvia are also used for the drinking water supply, but the amounts extracted are small as well. Water extraction from the rest of the unmentioned aquifers is performed only from individual water sources; therefore the amount of abstracted water is incomparably lower than the amount of the extracted water for the water supply of several towns or cities.

When looking back in the past, in the year 1950, the most used aquifers were the Quaternary and D_{2-3} Arukila – Amata multi aquifer. Water extraction from the other aquifers was insignificantly small. The same pattern was true in 1980 – the Quaternary and Arukila – Amata multi aquifer maintained the main role in water abstraction in Latvia. Comparing water abstraction data for 2000 and 2010, there was still a decrease in the total amount of abstracted water, but the main decrease was from the Quaternary aquifer. The main reason was that the Riga city needs less water and some portion of groundwater today is also provided from new wells in the Gauja – Amata aquifer. A very slight decrease in extracted water from deeper aquifers is also visible, but this may not be a true trend. One must take into account that this data may not be mirroring the exact true situation in nature, but only the general trend because of a lack of data in Latvia and further mathematical processing. Therefore, such a tiny difference should be counted as a mathematical processing error not as a true observable trend in nature.

The sources of groundwater in Estonia are more diverse, and fairly similar amounts are abstracted from several aquifers and multi-aquifers. In Estonia, in 2010, the most loaded aquifer was the Silurian (S) with 27000 m^3/day, where the major consumers were the cities in the south of Estonia – Tartu, Kuressaare, Viljandi, and the Cambrian – Vendian (C-V) aquifer with 22,000 m^3/day, where the consumers were the cities in the north of Estonia, including Tallinn. Similar amounts were abstracted from Vendian aquifers (V2gd, V2vr), Cambrian – Ordovician (C-O), Ordovician (O) and middle Devonian (D2), with around 10 thousands m^3/day. The Quaternary was (11,000 m^3/day) – Likewise in Latvia. The Quaternary aquifer was mainly consumed by the two biggest cities of Estonia: Tallinn and Tartu, with total abstraction about 11 thousand m^3/day. Looking at the multi aquifer systems, the main one was the Cambrian – Vendian multi aquifer, providing about 33% of the total amount of abstracted water and the Ordovician – Silurian multi aquifer providing 32% of the water.

In 1950, groundwater was abstracted only from the V2gd aquifer by Tallinn and other northern cities because this aquifer was located very close to the topological surface in the very northern part of Estonia. There was also a tiny amount of abstracted water from the aquifer C-V used by Tallinn. In the period 1950 – 1980 a rapid increase in water abstraction was observed, especially in aquifer C-V where the main water consumers were Tallinn (21,000 m^3/day); Kohtla-Järve (16,000 m^3/day) and the northern towns (27,000 m^3/day). There was also significant increase in aquifers V2gd mostly used by Tallinn; S mostly used by Tartu; Q mostly used by both – Tartu and Tallinn, and O-C mostly consumed by towns all over Estonia. After 1980 and until 2000, the abstracted water amount decreased in some of the main aquifers – V2gd, Q, and especially C-V where the abstracted groundwater amount for Tallinn was reduced 5 times; the abstracted groundwater amount for Kohtla-Järve – 3 times; the abstracted groundwater amount of the northern towns – 4 times, which may be explained by the crash of industry after the restoration of the independence of the Baltic countries.

The water supply in Lithuania, like in Latvia relies on few main aquifers and multi aquifers. The most loaded one is Quaternary aquifer, which is used for water supply of larger cities as Vilnius, Kaunas and other. About 200000 m^3 groundwater per day is abstracted nowadays, and it is four times more than from other main groundwater source – middle and upper Devonian Arukila – Amata multi aquifer (local aquifer name – Šventosios – Upninku). D2ar-D3am multi aquifer mainly is used in the central and northeastern Lithuania, and nowadays about 50000 m³ groundwater per day is abstracted. Other aquifers of upper Devonian, upper Permian and Cretaceous have subregional importance, nowadays contributing about 10-20 thousand m³ of groundwater per day. Comparing groundwater amounts abstracted in 1980 and 2010, there is significant fall observed. Groundwater amount abstracted from any of the aquifers used has decreased two times.

Groundwater abstraction and the hydrogeological regime

Based on an analysis of the changes in total groundwater abstraction amounts in time, three different hydrogeological regimes or scenarios of groundwater use may be distinguished:

1. the natural scenario, where there is minimal groundwater extraction, and hydrogeological conditions are close to the natural, undisturbed ones; the effect of groundwater extraction is nearly unnoticeable compared to the natural processes of water circulation (before 1950);
2. the wasteful scenario, where groundwater abstraction is very high, the natural hydrogeological conditions of the aquifers are disturbed; groundwater levels near the main abstraction sources are significantly lowered; the effect of groundwater use is clearly visible in the groundwater flow patterns (1965 – 1990);
3. the sustainable scenario, where groundwater abstraction is in reasonable amounts; the disturbed hydrogeological conditions of the previous scenario have returned to the semi-natural state; the effect of groundwater extraction is minimal, maintaining the restoration of the natural groundwater resource (after 1990).

The trend of groundwater extraction in all Baltic countries is similar – starting with 1950, until approximately 1965, the representative trend was minimal water extraction (natural scenario of groundwater extraction); from 1965 until 1990 the characteristic trend was an increasing amount of groundwater extraction, which leads to a wasteful scenario of groundwater extraction at the end of the given time period; after 1990, a rapid decrease in the amount of extracted groundwater was observed, referring to a medium scenario of groundwater extraction nowadays (Figure 3).

To understand the influence of these scenarios throughout history, the timeline of the observed piezometric water level in monitoring well No.689 (Jelgava district, Valgunde) of the upper Devonian Gauja aquifer (D3gj) has been shown in Figure 6. The rapid decrease in the water level of the monitoring well in the interval from 1982 until 1990, has to be proportional to the increasing amount of abstracted groundwater from the water supply wells. After the historical events in 1990, and the closing of most industrial factories the water level in the monitoring well increased to what is refered to as groundwater resource restoration. As well No.689 gives no data before 1982, this period is covered using data on the groundwater levels in the water supply wells at their installation date. The water level in wells within a radius of 4 km around well No 689 is shown.

The outlined scenarios were used for groundwater flow modelling in the BAB applying the developed modeling system MOSYS version 0 (Sennikovs et al., 2011, Virbulis et al., 2012). Steady state calculations were performed for each of the scenarios.

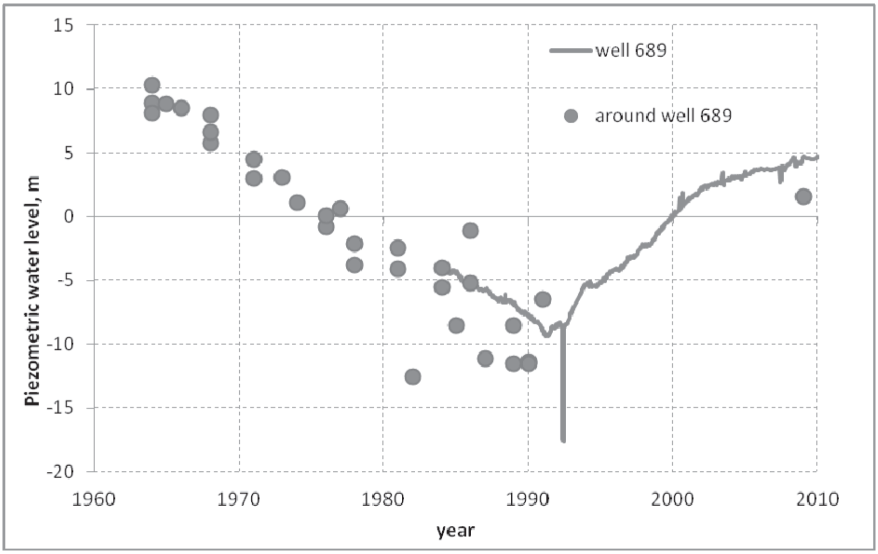


Figure 6. The timeline of the observed piezometric water level in monitoring well No. 689 (line) and the measured levels during installation of wells in a 4 km radius around well No.689 (dots) near Jelgava with a filter located in the upper Devonian Gauja aquifer (D3gj).

Modelling of the cones of depression

Intense and significant groundwater extraction, represented by the wasteful scenario, led to a serious decrease in piezometric levels in the most used aquifers, and cones of depression formed around the largest wellfields and groups of wellfields.

The usual non-homogeneous distribution of water abstraction wells throughout the BAB led to the existence of a limitation on groundwater usage. If the limit was exceeded, regions with lower piezometric water level were formed as compared to the case without any water extraction. As shown by the results of transient-state calculations using the hydrogeological model of the BAB version 0, groundwater extraction in Latvia and Estonia caused distinct areas of depression. In Latvia cones of depression were observed in the upper Devonian Gauja aquifer (D3gj), the upper Devonian Amata aquifer (D3am), the middle Devonian Burtnieki aquifer (D2br) near Rīga, Jelgava (Figure 7), and Liepāja in the upper Devonian Famenian multi-aquifer. In Estonia, depression cones were observed in the Cambrian aquifer near Tallinn and Kohtla-Järve, and in the Silurian aquifer near Tartu in cases of the wasteful scenario of groundwater abstraction. Nowadays, when the sustainable scenario of groundwater abstraction is considered, the water level in the areas of the cones of depression has been increasing, however the cones of depression have not vanished, but are not as pronounced as in 1990.

Figure 7a shows the modelled distribution of the piezometric head in the upper Devonian Gauja aquifer in 1900, when there were natural hydrogeological conditions and no water had been abstracted. The piezometric head isolines were formed as quite smooth except the area of Rīga city where the River Gauja and Lake Ķīšezers is taking a role in the displayed piezometric head. Contrary to the 1900, in 1990 (Figure 7b)

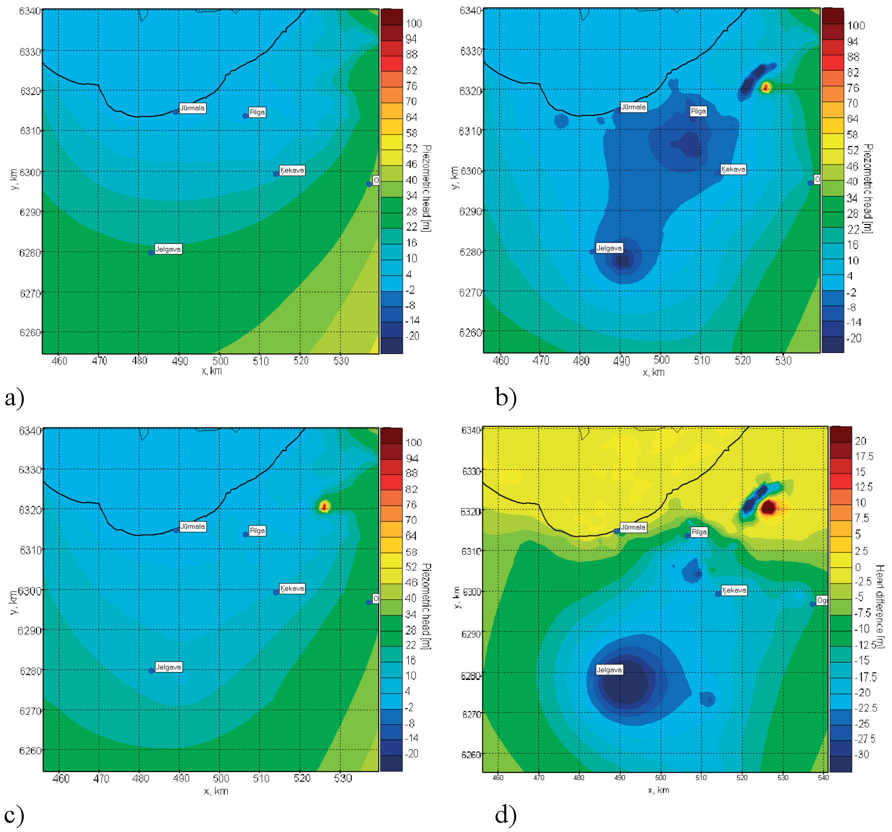
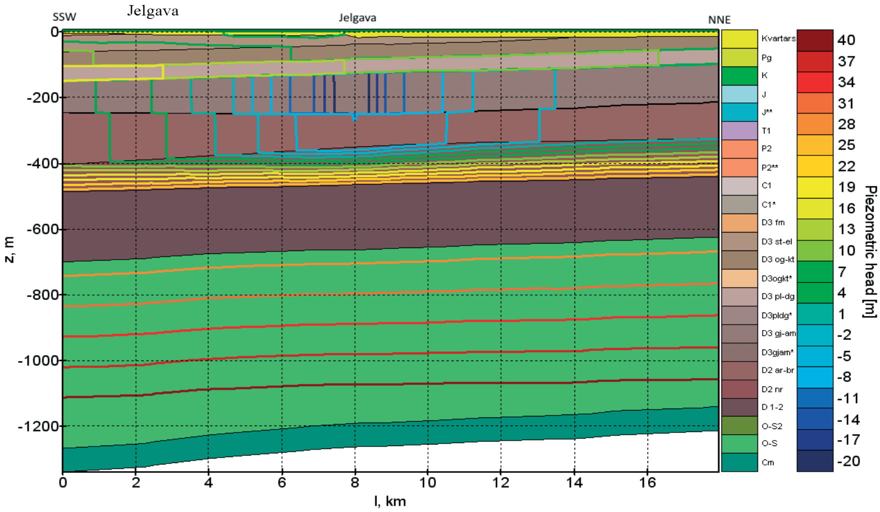


Figure 7. The modelled distribution of piezometric head in the upper Devonian Gauja aquifer (D3gj) in Riga and Jelgava surroundings. a) water abstraction in 1900; b) water abstraction in 1990, the dark blue areas show the cones of depression; c) water abstraction in 2010; d) The difference of the piezometric head in 1900 and 1990. The blue coloured areas correspond to the situation when the piezometric level in 1990 was lower than in 1900. The thick black line defines the coast line of the Gulf of Riga.

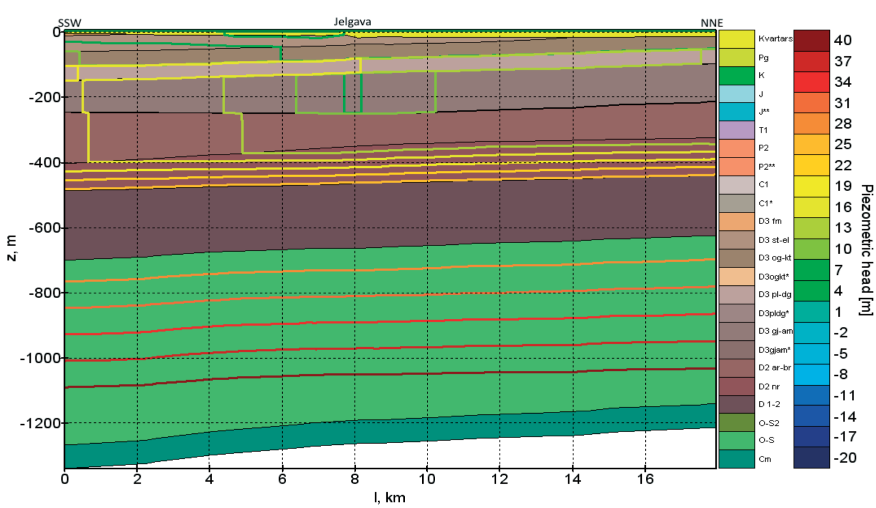
there was a rapid decrease in the piezometric water level observed in the areas near Jelgava, Rīga and Baltezers, where the groundwater for the water supply for Rīga had been extracted, as well as some smaller cones of depression in the area of Jūrmala City. The little red area near Baltezers shows the area of artificial recharge for the Baltezers wellfields. Figure 7c shows the distribution of the piezometric water level nowadays, in 2010. Compared to the piezometric head distribution in 1900, it is obvious that a semi-natural groundwater flow regime has been established. The water levels are lower than in 1900, but the general flow pattern with no obvious signs of depression cones is similar to the one in 1900. The comparison of modelled piezometric levels in 1900 and 1990 (Figure 7d) shows that the wasteful scenario had a more significant influence on the groundwater flow regime in the Jelgava area rather than in the Riga area, although the depression cone in the Riga area was deeper and wider.

For a better understanding of the influence of water abstraction on groundwater flow, it is useful to compare the modelling results for 1980 and 2010 in the vertical cross-section view. Figure 8 gives an example of a piezometric head distribution in the vertical cross-section near Jelgava.

Significant water abstraction (25-29 thousands m³/day) in the upper Devonian Gauja – Amata aquifer (D3gj+am) influences the adjacent aquifers like the middle Devonian Burtnieki – Arukila aquifer (D2ar+br). Groundwater abstraction of such an amount leads to a rapid fall in the piezometric water level (the area marked by dark blue lines in Figure 8a).



a)



b)

Figure 8. Distribution of the piezometric head in the vertical cross-section near Jelgava in 1980 (a) and 2010 (b). Coloured lines depict the modelled piezometric head. The blue area in 8a shows the depression cone formed due to significant ground water abstraction in 1965-1990. The light green area in 8b shows the current cone of depression formed as a result of groundwater abstraction nowadays.

The head difference between Gauja – Amata aquifer and the upper lying Plavinas – Daugava multi aquifer separated by a thin aquitard is about 40 m thus facilitating groundwater leakage from the above aquifers. The steep gradient between the Arukila – Amata multi aquifer and the lower and middle Devonian aquifer also facilitates leaking of groundwater from the lower aquifers. In 2010, in the case of the sustainable scenario of groundwater abstraction, the head difference between D3pl-dg and D3gj+am is 10 meters (Figure 8 b) and the influence on the groundwater flows is negligible. Figure 8 also shows that water abstraction on shallow layers has no influence on the groundwater flows in the deeper aquifers of the BAB, nevertheless this is the water abstraction scenario.

The role of the hydrogeological model of the BAB in groundwater management

To ensure the sustainable usage of groundwater resources of the BAB, studies should have been performed to find out the impact of the investigational scenario of groundwater abstraction in a long term period. Therefore, the BAB model version 1 was used (Virbulis et al., 2012b) which is suitable for steady-state calculations predicting the steady-state distribution of the piezometric water level with a given amount of water abstraction.

The results of a steady-state calculation for the wasteful scenario of groundwater abstraction, where the water extraction sources and amounts for 1980 (Figure 4) have been used, are considered at first. The calculations show that if such an amount of water is extracted for quite a long time, depression cones will be deeper. In the areas of Rīga and Jelgava (Figure 9), and Tallinn the limit of groundwater resources may be reached. There is also a risk of the formation of large depression cones in the upper Devonian Amata aquifer (D3am) in the Latvian cities of Liepāja and Jēkabpils as well as in the upper Vendian (V2) aquifer in the Estonian city of Kohtla-Järve.

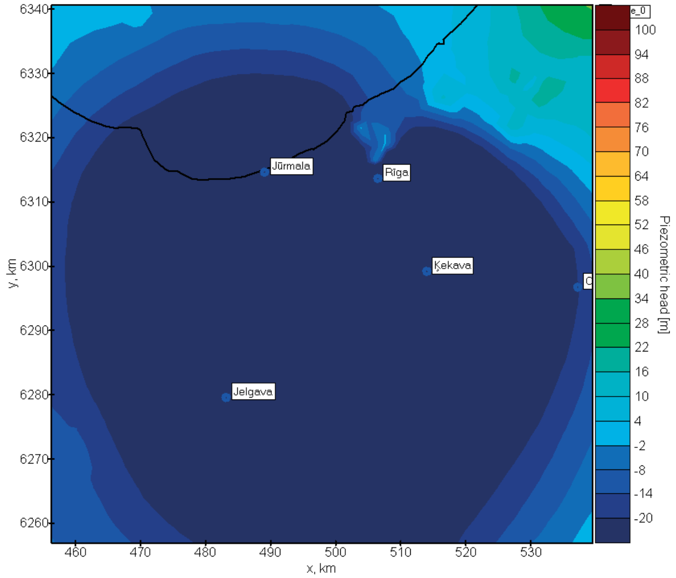


Figure 9. The distribution of the modelled piezometric water level in the upper Devonian Gauja aquifer in steady state conditions for the wasteful scenario of groundwater abstraction (abstraction data on 1980).

Figure 9 shows an example of a predicted cone of depression in the area Rīga-Jelgava in the upper Devonian Gauja aquifer (D3gj) based on steady state calculations. Comparing Figure 9 with Figure 7b, it is obvious that the area of the cone of depression has increased to an extreme degree, and the piezometric head is barely above the top of the aquifer. The model results also prove that water abstraction in accordance with the wasteful scenario will in the long-term cause serious problems with groundwater resources. Actually, in the case of Latvia, these problems were already observed at the end of 20th century, when a depression cone of a maximum radius of 100 km around Riga was formed (Levins et al, 1998).

In taking a look at the results of stationary calculations of the sustainable scenario of groundwater abstraction, where the water extraction sources and amounts for 2010 (Figure 10) were taken, one can observe some mild changes in the distribution of the piezometric water level.

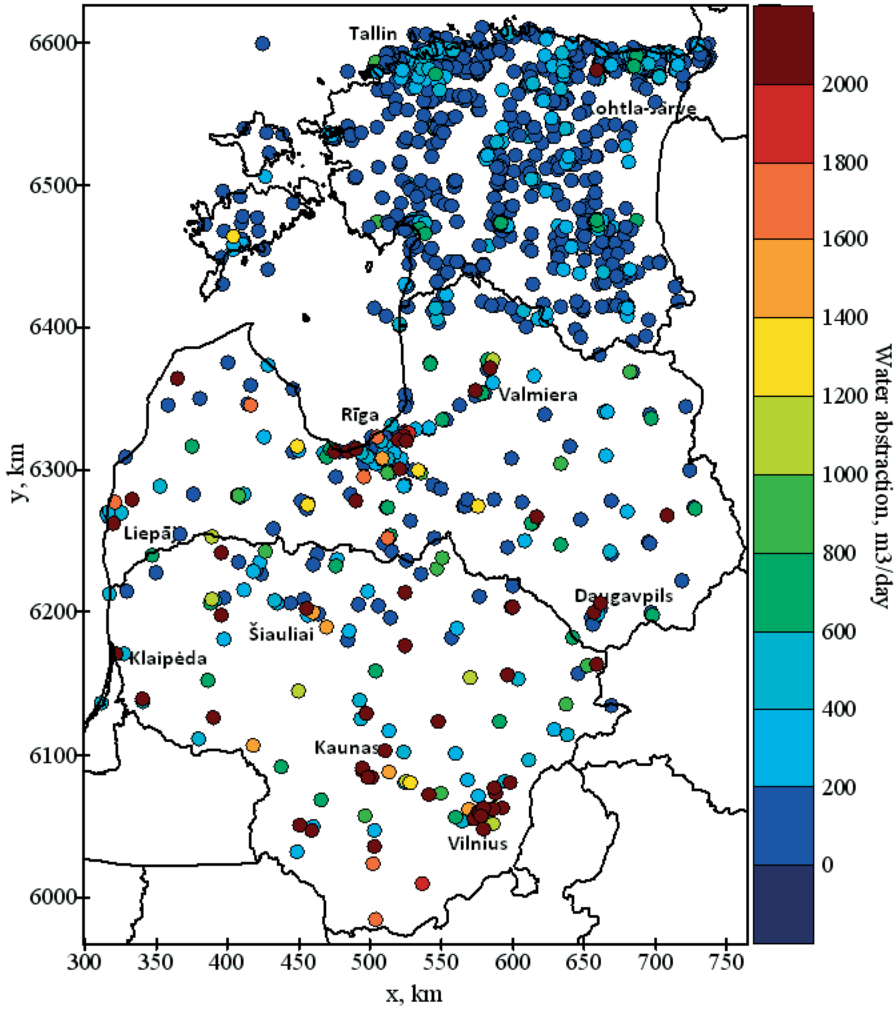


Figure 10. Map of groundwater extraction sources and amounts in 2010.

Steady state calculations using the water abstraction data of the sustainable scenario show that the depression cones will be slightly deeper than in the transient state conditions. The largest cones of depression still remain in the area of Rīga-Jelgava in the middle Devonian Arukila – upper Devonian Amata multi aquifer system (Figure 11), and in the area in the north of Estonia with Tallinn and Kohtla- Järve pumping the water from aquifer V2. The steady state calculation results for the sustainable scenario of water extraction do not show the formation of any other significant cones of depression in any other cities.

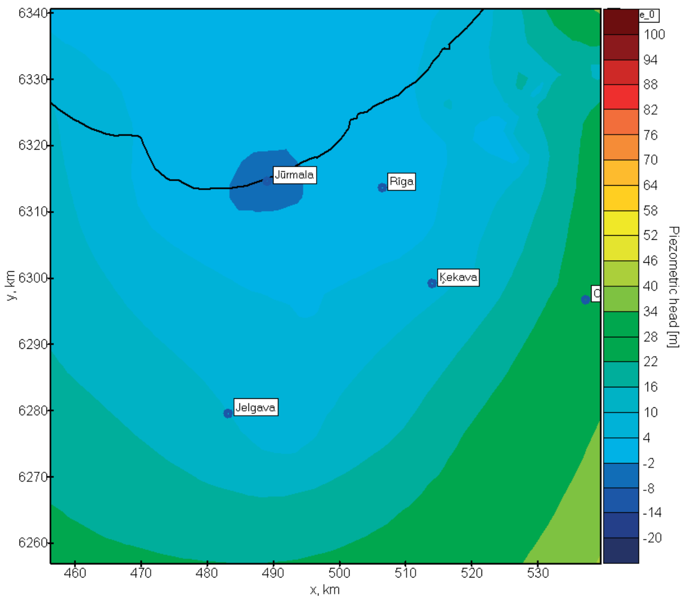


Figure 11. The distribution of the modelled piezometric water level in the upper Devonian Gauja aquifer in steady state conditions for the sustainable scenario of groundwater abstraction (abstraction data for 2010).

Conclusions

Although the compiled data sets on groundwater abstraction in Latvia, Lithuania and Estonia lack some accuracy, the data analysis performed here provides a general view on the development of groundwater use patterns in the BAB.

Groundwater abstraction in the BAB has changed in time and space, but the trends of the changes are rather similar for all Baltic countries. The most typical pattern is as follows:

- very low groundwater abstraction before the year 1950,
- a slow increase in abstracted groundwater amounts and number of wells in 1950-1965,
- a rapid increase in the extracted groundwater amount and the number of wells in 1965-1990, with the exception of Latvia, where extensive groundwater use ceased in the 1970's due to the overexploitation of groundwater resources in the upper Devonian Gauja – Amata aquifer in Riga and surroundings, causing stabilization of groundwater use in 1975-1990,

- a sharp decrease in the extracted groundwater amount in s 1990-2000 and
- a slow stabilization of groundwater abstraction since 2000.

Based on the modelling results it could be concluded that the current groundwater abstraction amounts are sustainable and will maintain reasonable fresh groundwater resources in the long-term. A significant increase in groundwater abstraction in any location and from any main aquifer used for water supply should be analyzed in detail to avoid a loss of fresh groundwater resources.

Acknowledgements

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Oxygen and hydrogen stable isotope composition in the groundwater of the Baltic Artesian Basin

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Abstract

This paper tends to give a general overview of groundwater diversity in the Baltic Artesian Basin from isotopic content point of view. In this study major emphasis put on water stable isotope investigations and their history in the region attempting to solve issues of main mechanisms and conditions of groundwater recharge in the region. Results show that groundwater recharged mainly during the Holocene, however in the northern part of the basin glacial melt water with depleted up to – 22 δ18O‰ VSMOW stable oxygen values can be found, however in the deepest aquifers of the Baltic artesian basin much more enriched isotopic values are common, ratios are up to only -4,6 δ18O‰ VSMOW. It is observed that measured stable isotope ratios are more depleted in the northern part of the basin, at the same time in similar depths towards southern margins it much less depleted. It is also characteristic that increased salinity and aquifer depth is associated with more enriched stable isotope values.

Keywords: water stable isotopes; groundwater; recharge conditions

Introduction

Isotopes are atoms of the same element that have different numbers of neutrons but the same number of protons and electrons. The difference in the number of neutrons between the various isotopes of an element means that the various isotopes have different masses (Drever, 2005). Recently more than 200 stable and more than 1,700 radioactive element forms of the 80 chemical elements have been discovered. The majority of chemical elements have at least one stable isotope. Many elements have two or even more stable, naturally occurring isotopes. In general, nuclei with even numbers of protons or/and neutrons are more stable (Clark and Fritz, 1997). The stable isotopes have nuclei that do not decay to other isotopes on geologic timescales, but may themselves be produced by the decay of radioactive isotopes (Drever, 2005).

From a hydrogeology point of view, water stable isotopes i.e. stable nucleons of oxygen (oxygen-16, oxygen-17, and oxygen-18) and hydrogen (protium, deuterium) are of the most importance, as these elements form water molecules and their ratios are less affected during the dissolution of compounds or atom exchange (Clark and Fritz, 1997). As well as water isotopes, more stable isotopes such are carbon, chlorine, sulphur, nitrogen, barium, lithium etc. are also widely used in hydrogeological studies although they are used in the more local studies to solve specific issues. Usage of non-water stable isotopes is limited by their possible absence in groundwater or their occurrence in negligible quantities.

As decay processes don't affect stable isotope ratios, there is no limit of age, physical parameters or concentration of any chemical component in the analyzed water. Therefore, a stable isotope approach can be applied to prescribe small scale groundwater systems thus solving issues of a small scale as well as characterizing regional groundwater systems with very variable residence times.

The stable isotope technique is an indirect method to determine groundwater age or resistance time in the subsurface, and oxygen and hydrogen isotopes are generally used to determine the origin of groundwater i.e. the conditions under which groundwater has been recharged.

Nevertheless, this technique has several limitations, and can't be treated alone. When large aquifer systems or even artesian basins are examined, it is crucial to apply other direct or indirect approaches for determining the age and residence time of groundwater. If large aquifer systems are examined additionally in a geological setting, hydrogeological conditions and even the evolution of large groundwater systems need to be investigated to get a more realistic reconstruction of recharge/discharge rates, territories and most importantly residence times in the subsurface.

Groundwater isotope studies in the BAB

Stable isotope application in groundwater studies in the Baltic Artesian Basin (BAB) started in Estonia in the early 1980's. The Institute of Geology in Tallinn has been investigating stable isotope signals in surface as well in sub-surface waters since 1976 (Punning et al., 1987). Extensive groundwater sampling for radiocarbon, stable carbon and stable oxygen content has been made in the territory of Estonia by (Punning et al., 1987; Vaikmäe et al., 2001; Karro et al., 2004; Marandi et al., 2004; Raidla et al., 2009; Raidla, 2012). The most available stable isotope data about Estonian groundwater was published by Raidla et.al. in 2012, however, most of the samples in Estonia represent mainly the Cambrian-Vendian multi aquifer system, as this particular aquifer system is of the most importance in north Estonia. Since then a significant data set has been collected mainly from groundwater; stable isotope ratios in other natural waters have been analyzed as well.

With respect to other parts of the Baltic Artesian Basin, stable isotope studies will be elaborated on much later. In Lithuania, the first data was published by Mokrik et al. in 2008, however, samples have been collected since 1985. In Lithuania, major emphasis was put on radiocarbon, tritium and other radioactive isotopes. Most studies there are devoted to the Upper Devonian aquifers, as in the southern part of the Basin, these aquifers are widely used in water supply for domestic and industrial needs.

Limited isotopic studies of groundwater in the central part of the basin were conducted – in Latvia – until recently. According to a paper by Mokrik et al. 2009 nine isotope samples were taken as well from different aquifers in the Latvian part of the basin in 1987 and 2000. However, a significant data set of groundwater stable isotopes in Latvia was produced during 2010-2012 within the framework of the ESF project "Establishment of interdisciplinary scientist group and modelling system for groundwater research." The content of ^{18}O, D, T, ^{13}C and ^{14}C in groundwater were measured over the entire territory and all the significant aquifers in the country.

The present paper is based on the results of 385 groundwater samples obtained from published data from Lithuania, partly published data from Estonia and unpublished data in the territory of Latvia. The locations of the collected samples and sampled aquifers are illustrated in Figure 1. It should be noted that most samples were analyzed only for stable oxygen ratios. However, only an insignificant number of deuterium measurements were done before 2010.

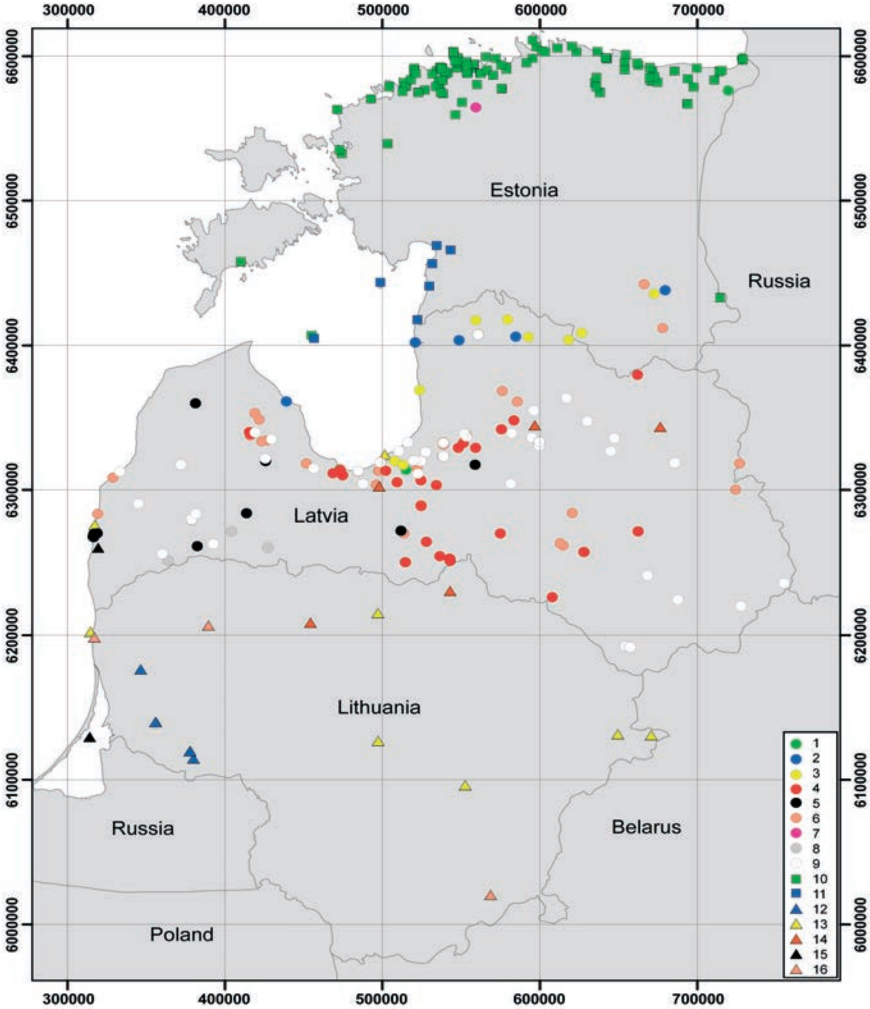

Figure 1. Stable oxygen and deuterium groundwater sampling sites (Raidla et al., 2012; Mokrik et al., 2009). 1-9: samples collected during the PUMA project, (were 1-Cambrian; 2 –Lower-Middle Devonian; 3 – Middle Upper Devonian; 4 – Upper Devonian sandstones; 5 - Upper Devonian carbonates; 6 – Famenian; 7 – Ordovician; 8- Permian; 9 - Quaternary); 10-11: samples from the Institute of Geology at the Tallinn University of Technology (were 10 – Cambrian; 11 - Lower-Middle Devonian); 12-16: samples published by Mokrik et al., 2009 (were 12- Lower-Middle Devonian; 13 - Middle Upper Devonian; 14 - Upper Devonian sandstones; 15 - Upper Devonian carbonates; 16 – Famenian).

$\delta^{18}O$ and δD values in precipitation

Groundwater recharge, especially the shallower embedded is predominantly of meteogenic origin; therefore, nowadays it is essential to identify the isotopic signal in precipitation and its spatial and seasonal variability.

For the Baltic States, stable isotope values in precipitation are available from the early 90's for the central and northern part of the Basin. However, the data set is sparse and doesn't represent all of the study area. A considerable amount of stable isotope data from precipitation was collected during Soviet times from the Riga meteorological observation site, during 1980-1988 and is available in the GNIP database maintained by the International Atomic Energy Agency (IAEA, 2006). Nowadays it provides important data about isotopic signal recharging from precipitation. According to these monitoring data, the precipitation long term mean weighted values of meteoric water are -9.74 $\delta^{18}O$‰ VSMOW and -72.6 $\delta^{2}H$‰ VSMOW respectively, and the mean calculated deuterium excess is 11.2. Seasonal fluctuations are less than 5 ‰ for $\delta^{18}O$‰ and 63 ‰ for δD‰ (IAEA, 2006). It is characteristic that values are more depleted during the cold season i.e. the values are more negative; however, there are more less depleted values in summer. A similar seasonal pattern can be drawn from precipitation monitoring data in the northern part of the Basin. The long term mean annual $\delta^{18}O$ values in contemporary precipitation in Tallinn, Estonia are estimated at –10.4 ‰ (Punning et al., 1987). However, the mean values between winter and summer months are in the range of 7 ‰ for $\delta^{18}O$‰. Precipitation samples for isotope analysis were taken from the Koosa weather station in east-south Estonia during the observation period from 1976 to 1984 (Punning et al., 1987).

It is well known that the spatial distribution of the isotopic signal in precipitation is regulated by several mechanisms, such as latitude, altitude effect, continentality and the origin of dominant air masses in the region (Aggarwal et.al., 2005). According to IAEA studies (IAEA, 2006) the major effect on the precipitation signal in the Baltic Artesian Basin is latitude, and more depleted values can be observed in the northern part of the basin, while there should be a less depleted input signal above the southern part of the Baltic Sea.

Seasonal fluctuations were observed: a summer maximum, winter minimum and close to mean values were detected in the fall and spring. Additionally, each rainfall event has its own isotope signature, therefore usually only mean monthly values are used. Taking into account the fact that groundwater recharge is larger during the spring and fall, the precipitation signal of the autumn and spring months should reflect groundwater mean values best.

Other natural waters, for instance surface water bodies, shift to less depleted values compared to precipitation and groundwater values which can be explained by fractionation during evaporation and in the case of the Baltic Sea, additional refreshing from the Atlantic Ocean, have a large impact. In west Estonia water samples from eleven lakes were analyzed in different seasons and the values were in a range between -11 and -3.6 ‰. There were slightly more negative values during the cold season. However, seasonal variations for particular lakes aren't that significant and stay more or less constant throughout the year (Punning et al., 1987).

$\delta^{18}O$ and δD values in the groundwater of the Baltic Artesian Basin

In the case of the Baltic Artesian Basin, it is characteristic that deeper parts of it have a larger protection level due to the fact that, a more likely older and less refreshed groundwater component can be found there. Marginal parts of the northern as well as the south-eastern edges are less protected and distinct groundwater sources (end-members) can be identified there.

Groundwater in the upper aquifers represents stable isotope values characteristic of precipitation in today's climate and depending on the recharge season and recharge area, varies in a wide range. It is common in a whole cross section that less depleted $\delta^{18}O$ values are found in the southern part, however, more depleted $\delta^{18}O$ values are found in the northern part of the basin. Major multi-aquifer systems and a range of values are represented in Table 1.

Table 1. Approximated description of major aquifers in the BAB (Raidla et al., 2012 and Mažeika et al., 2009)

Aquifer system	Northern part (Estonia)	Central part (Latvia)	Southern part (Lithuania)
	^{18}O values	^{18}O values	^{18}O values
Cambrian – Vendian	-18.1 to -22.9	-4.6 to -5.3	x
Cambrian - Ordovician	-11.4 to -18.9	X	x
Ordovician	-11.7 to -12.2	X	x
Lower-Middle Devonian	-10.9 to -12.6	-10.9 to -12.3	-4.5 to -9.9
Middle Devonian	-10.7 to -11.8	-10.7 to -13.4	-9.6 to -12.6
Upper Devonian (sandstones)	-11.1 to -11.3	-10.2 to -13.2	-11.7 to -13
Upper Devonian (carbonates)	x	-9.4 to -12.2	-10.4 to -12.2
Quaternary	x	-8.6 to -12.3	-10.4 to -11.7

With increasing depths i.e. below the regional aquitard, the composition of oxygen stable isotopes is in a much broader range.

In the northern part of the Baltic Artesian Basin, the Cambrian-Vendian aquifer contains very light i.e. much depleted, isotopic composition and the water is fresh, mainly Na-Ca-Cl type, while towards the south salinity increases and the values are getting less depleted, but the Na – Cl type remains. The origin of fresh groundwater in northern Estonia is well examined, however, the origin of Na-Cl type brines are still the subject of discussion.

Similar spatial regularities can be observed in the Lower-Middle Devonian aquifers, where fresh Ca-HCO_3 water zones contain more depleted waters compared to Na-Cl type waters, and where higher mineralization means a shift towards positive values.

Groundwater occurring in the Middle and Upper Devonian sediments above the regional Narva aquitard were more likely formed during different Holocene stages, and delta ^{18}O values are in the range of -13.4 to -9.6 ‰ with more depleted values observed in the central part of the basin and less negative values in the southern part.

Adjusted carbon-14 ages show that modern recharge water is spread in the Quaternary and Lower Frasnian aquifers from several tens to 90 meters, for the Middle Frasnian – from several to 24 meters and for the Upper Eifelian-Givetian aquifer, 90-185 meters correspondingly. Along the down gradient flow path in the diapason of 40-250 meters, the groundwater age increased progressively up to 20,000-25,000 years BP, except with many samples from the Middle Frasnian aquifer, where the old age of water was considered with the dedolomization of water-bearing rocks adding a lot of very old DIC near the surface. In the areas of groundwater up-gradient flow the age distribution along depth has a reverse character, due to vertical leakage through tectonic lineaments and river valleys towards the surface. Old groundwater in the river valleys and in the vicinity of hydraulically permeable tectonic fractures is confirmed by the location of geogenic helium anomalies (Mokrik, 2003; Mokrik et al., 2002).

When all delta oxygen-18 values are plotted versus depths, unambiguous interpretation can be done. In the lowest Cambrian aquifers, several groundwater end-members can be distinguished with significantly depleted delta oxygen-18 values for groundwater of glacial origin in northern Estonia and brines with a shift towards positive values (Fig.2 (A)). Similarly the Lower-Middle Devonian aquifer has two different directions. One goes towards more negative values with increasing depth and the other towards more positive values.

A similar pattern is drawn when delta values are plotted versus chloride concentrations, which suggests that more likely the mid values are the result of mixing between these two end-members (Fig. 2 (B)).

From the relationship between deuterium and oxygen-18 values, it is possible to find out the processes which impacted stable isotope composition after infiltration, such as secondary evaporation and intensive interaction with the matrix etc. (Aggarwal et.al., 2005). The trend line in Fig.2 (C) is constructed from precipitation data from the Riga meteorological observation station (IAEA, 2006). Most groundwater samples are slightly shifting around the constructed trend line, which indicates minor isotopic changes after infiltration into the aquifer. It was also observed that the local meteoric line is less characteristic to shallower embedded aquifers and there is better matching for aquifers below the Upper Devonian aquifers. It should also be emphasized that even glacial melt water from the Cambrian-Vendian aquifer in Estonia is plotted on the constructed local meteoric line (Fig. 2 (C)).

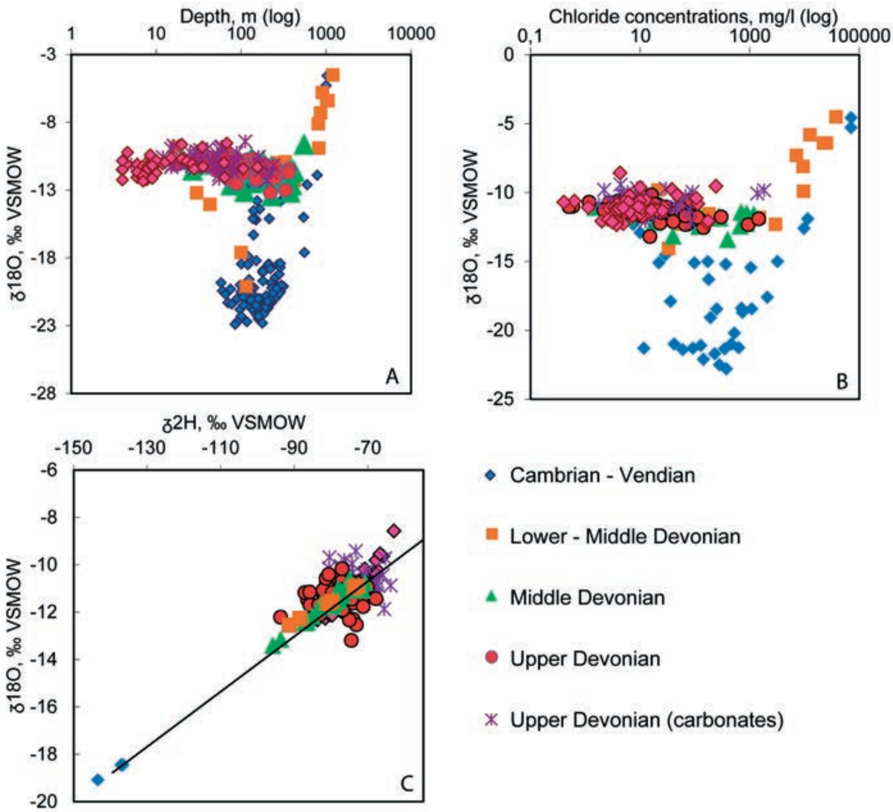

Figure 2. Stable isotope ratios of different aquifers in the Baltic Artesian Basin versus depth of sample (A), chloride concentrations (B) and delta deuterium (C).

Case-studies

Stable isotope technique is a valuable tool too in solving issues of particular aquifers or spatial anomalies; therefore, they were used in various studies throughout the Baltics.

As the Cambrian-Vendian aquifer system is the most important source of public water supply in northern Estonia it has been intensively studied at various times over the last decades (Yezhova et al., 1996, Mokrik, 1997; Perens and Vallner, 1997, Vaikmäe et al., 2001, Marandi et al., 2004, Karro et al., 2004, Vaikmäe et al., 2008, Raidla et al., 2009).

Many works are accomplished in northern Estonia to solve the issue of fresh water intrusion in the Cambrian–Vendian aquifer. The glacial origin of the groundwater in the Cambrian – Vendian (Cm-V) aquifer system of Estonia has been suggested by Punning et al. (1987) and Vaikmäe et al. (2001). Both suggested that glacial meltwater with a more negative ^{18}O composition of -22% intruded the Cm-V aquifer system, but in the work by Vaikmäe et al. (2001), the noble gas analyses allowed to conclude, that palaeorecharge took place at temperatures around freezing point (Edmunds, 2001).

In northern Estonia, the most characteristic feature of the Cambrian-Vendian aquifer system is the very light oxygen isotopic composition ($\delta^{18}O$ values from –18 to –22‰) of the groundwater, which provides an ideal tracer for the detection of possible changes in groundwater baseline quality. Around the ancient buried valleys, the intrusion of fresh groundwater from overlying aquifers and/or rainwater to Cambrian-Vendian aquifer system can occur. The intensity of such fresh water intrusions varies spatially and temporally, depending on the extent of groundwater exploitation near the valleys. In areas where groundwater drawdown is significant, freshwater intrusions occurs into the aquifer through the buried valleys and cause the groundwater chemistry and its isotopic composition to change. The δ18O values are usually higher than -15 ‰ due to freshwater intrusions and the TDS contents are low (200–500 mg l–1).

An investigation of groundwater with brackish composition in the Nemunas River Valley in the environs of Birštonas town, which is in the southern part of the Baltic Artesian Basin was supported by carbon and oxygen isotopes (^{14}C, ^{13}C, ^{18}O), tritium (^{3}H) and helium ($^{3}He + {}^{4}He$) studies in the last decade. The $\delta^{18}O$ values of groundwater attributed to the Triassic and Cenomanian-Upper Cretaceous multi-aquifers in the Birštonas area change from –10.7 to –9.4‰ which is close to the oxygen isotope composition of contemporary precipitation and indicates groundwater recharge in the post-glacial time (Zuzevičius, et al., 2007).

During the construction and operation of the Ignalina Nuclear Power Plant, which is located in the recharge zone of the eastern part of the Baltic Artesian Basin, the ^{14}C, ^{3}H content and to a lesser extent the $\delta^{13}C$ and $\delta^{18}O$ values were determined in groundwater attributed to the Quaternary and Upper-Middle Devonian multi-aquifers. The $\delta^{18}O$ values of groundwater for this area vary from -11.1 to -10.8‰ (Juodkazis, 1995) which indicates groundwater formed in modern recharge conditions.

The water of Lake Drūkšiai was used for the cooling of the Ignalina Nuclear Power Plant, and it was therefore a subject of extensive isotope research as well (Mažeika and Taminskas, 2005). The water balance of the lake and the interaction between the surface water and groundwater in the catchment was evaluated applying an extensive isotope data set. The oxygen isotope composition of groundwater in the area of Lake Drūkšiai attributed to the active exchange zone changes from –11.9‰ to –9.0‰ (Mažeika et al., 1999). The most negative $\delta^{18}O$ values are characteristic of the western part of the Lake Drūkšiai area and together with the highest piezometric level of groundwater, indicate a recharge zone. The most positive $\delta^{18}O$ values are characteristic of the eastern part of the Lake Drūkšiai area close to the tectonic fault zones where the piezometric level distribution in consequent aquifers shows groundwater leakage through confining beds from deeper aquifers to the subsurface. These areas have been qualified as regional discharge areas with relatively positive $\delta^{18}O$ values in the Upper-Middle Devonian multi-aquifer (Middle Lithuania) (Mažeika and Taminskas, 2005).

Investigation of a salty water anomaly in Birštonas and Druskininkai situated in the southern part of Lithuania, indicates that the fresh groundwater had mainly been formed in the Post-Glacial time (Holocene) $\delta^{18}O$ ranging from -11.5 to -8.8 ‰ SMOW, and differing very slightly from the average for meteogenic water. This was confirmed by radiocarbon dating showing the fresh groundwater age as usually being less than 10,000 years (Zuzevičius et.al., 2007).

A year-long monthly observation of the stable isotope composition of groundwater from various aquifers as well as surface water at Plavinu hydropower plant (HPP) was conduced to investigate the groundwater sources. Stable water isotopes fluctuate seasonally in the reservoir while remaining stable throughout the year in groundwater, i.e. the monthly variation is less than 0.5 ‰. The mean values of the shallower embedded carbonate Upper Devonian aquifer and the deeper embedded Middle-Upper Devonian aquifer differ by more than one per mill with more depleted values in the deepest aquifer. This indicates either the presence of groundwater recharged in colder climate conditions or a major recharge area situated in higher altitude, for example, the Vidzeme highland (Babre et.al., 2012).

Summary

The history of stable isotope studies in the groundwater of the Baltic Artesian Basin goes back more than 30 years, and was begun at the Institute of Geology, where major facilities for such analysis are located and all groundwater samples from the Baltic States are measured. Since 1976, a considerable number of samples have been collected throughout the Basin and from most of the aquifers present in the area. However, some areas have been much better studied and areas still uninvestigated remain.

Historical precipitation data from two observation stations is available, however, only one contains both i.e. isotope analyses. Both meteorological stations aren't situated in the most representative places either and present the marine climate more. Therefore, no data from the main groundwater recharge areas is available i.e. from highlands.

Until 2010, most groundwater samples were measured only for oxygen-18, but later deuterium was also measured in all groundwater samples.

Stable $\delta^{18}O$ in the groundwaters of the Baltic Artesian Basin is in the range of -22 ‰ up to -4.6 ‰, however, the majority of samples tend to shift around -11‰ $\delta^{18}O$ which slightly differs from the mean $\delta^{18}O$ values in precipitation. The most depleted and most enriched heavy oxygen values are situated in the Cambrian-Vendian aquifer system. Therefore, groundwater of different origin occurs in the same aquifer, which is apparent from a chemical composition point of view as well.

In the northern part of the BAB, three groundwater end-members can be distinguished: fresh and isotopically depleted $\delta^{18}O$ composition glacial melt water of Weichelian Ice Age, mainly in the Cambrian-Vendian aquifer, Na-Ca-Cl composition basin brine with less depleted isotopic values of unknown age and modern meteoric water with a stable isotope signal close to nowadays precipitation.

In the central part of the basin, fresh Ca-HCO_3 and Ca-SO_4 types predominate in the upper aquifers where groundwaters have a stable isotope signal similar to nowadays precipitation, around -11‰ $\delta^{18}O$. With increasing depth, the isotopic signal becomes more depleted, however, it does not exceed -13.4 ‰ $\delta^{18}O$, and these waters are mostly the fresh Ca-HCO_3 type or brackish Ca-SO_4 or Na-Cl type. However, in the deepest embedded aquifers, TDS significantly increases, the dominant groundwater type is Na-Cl and the stable isotope values become significantly more enriched in oxygen-18.

In the southern part of the basin, groundwaters of modern recharge can be found in the upper part. Groundwaters of Holocene age predominate down to 600 m depth.

In the western part of the basin it was determined that groundwater recharge in Devonian aquifers took place during the last ice age as well, however, the stable isotope composition is far less depleted than in the northern part and does not exceed -13.1‰ $\delta^{18}O$. In the southern part as well, Na-Cl brines with much enriched oxygen-18 values occur, however they are situated in the Lower-Middle Devonian aquifer.

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Impact of climate change on the shallow groundwater level regime in Latvia

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Abstract

The annual regime of shallow groundwater levels significantly impacts agricultural and forestry production. To adapt to the climate changes it is necessary to know the possible changes in the annual regime of shallow groundwater levels. The aim of this paper is to model the annual regime of shallow groundwater levels using an ensemble of eleven climate projections according to the dominance of continental and oceanic air masses in Latvia. The observed and modelled long-term mean monthly groundwater levels for the reference period (1961-1990) and a future period (2071-2100) are transformed into relative values and analyzed. The METUL mathematical model was chosen as a known and appropriate model for Latvian climate conditions to model future ground water levels using meteorological data. There are significant differences in the groundwater regime between the reference and the future periods and between the different members of the ensemble of climate projections. Statistical methods focusing on percentile analyses were used to characterize the variability of different climate scenarios on the annual regime of shallow groundwater levels. The results shows the probability of relative groundwater levels for a future period (2071-2100) by climate scenarios according to the dominance of continental and oceanic air masses in Latvia.

Keywords: Climate change; hydrological year; continentality; groundwater modelling; METUL

Introduction

Groundwater systems are dynamic and adjust continuously to short-term and long-term changes in climate, groundwater withdrawal and land use (Genksu et al., 2005, Duchan et al., 2008). Groundwater level fluctuations are important, firstly for environmental protection: for maintaining the groundwater equilibrium system, controlling groundwater level fluctuations and protecting against severe land subsidence (Kumar and Singh, 2010). Secondly, for agriculture and forestry industries as water is one of the resources on which sustainable yield quality and quantity is dependent (Schleyer, 1994). These fluctuations can be described over a long-term period, separated by hydrological year and averaged per month creating a specific shape function, which represents the groundwater level fluctuation regime.

The classical Latvian long-term groundwater level fluctuation regime is described as an M-shaped function which represents two groundwater level maximums and minimums. The first and major maximum occurs in spring (April) when, in addition to the snowmelt, rainfall enhances surface runoff and boosts groundwater recharge. Accordingly, this maximum is called the spring maximum. In the summer, the developed vegetation cover combined with higher temperatures, increases evapotranspiration, and the groundwater levels decrease reaching their major minimum in August, called the summer minimum. Starting from September, in the autumn months, groundwater levels tend to increase due to frequent rainfalls and slowly decreased evapotranspiration. The second maximum occurs at the beginning of winter (December) and is called the autumn maximum. Due to the low temperatures and frozen soil surface during the winter months, the groundwater levels tend to decrease reaching the winter minimum in February and is called the winter minimum (Толстов, 1986).

Latvia is situated within the transitional zone between the oceanic north-western part of Europe and the continental north-eastern part of Europe; between the oceanic or maritime part and the interior regions of Europe. It has a vast area of flat plain-land without any natural barriers to air mass movement. This results in high daily variability, diversity and inter-annual changes in the air mass frequency. The annual course of recurring air mass combinations, as well as the cycle of net radiation, near-surface temperature, amount of precipitation, elements of water balance and phenological phenomena all have explicit seasonality. The mapping of the degree of climatic continentality, describing it with the Conrad coefficient has been done previously (Draveniece, 2007). Continentality describes the climate of areas influenced by air masses over large continental or oceanic bodies. Such an assumption suggests that in Latvia the monthly groundwater level varies spatially depending, not only on climate conditions in general, but also on one particular climate characteristic – continentality. The objectives of this paper are 1) to analyze the spatiotemporal patterns of the long-term mean monthly groundwater levels in Latvia in two different time periods according to the spatially changing degree of climatic continentality and 2) to highlight the significance of climate change impact on the groundwater level regime.

The impact of climate change has been widely studied in different hydrological research areas, for example, in water resources management and sustainability (Gupta, 2010) and flood risk management (Gouldby, 2008).

In this study, the groundwater level fluctuation regime was analyzed in a future period (2071-2100) within 11 different climate projections derived from A1B scenario. The METUL groundwater model (Krams and Ziverts, 1993) was used to model groundwater levels for all projections. There are several groundwater models, which calculate daily groundwater levels from meteorological data (Bergström, 1995), but the METUL model was chosen as the best known and most appropriate model available by the group of authors.

Materials and methods

Data collection and verification

Water-level measurements from observation wells are the principal source of data. Long-term, systematic measurements of water levels provide essential data needed to evaluate changes in the resource over time, to develop groundwater models and forecast trends, and to design, implement, and monitor the effectiveness of groundwater management and protection programs (Houston, 1983). Shallow groundwater levels in Latvia have been actively monitored since the 1960's (Levina et al., 1998). In this study, groundwater levels were modelled based on the wells calibrated in the previous research (Lauva et al., 2012), where data was obtained from the well and groundwater level database of the Latvian Environment, Geology and Meteorology Centre that met the following conditions: (a) the groundwater level time series covers the time period from 1961 till 1990, (b) the depth of the well filter is less than 10 meters from the ground surface and the filter is penetrating highly conductive sand, (c) the data collection frequency for the selected well is less than seven days, (d) the groundwater minimum water table resides no deeper than 3 meters from the ground surface.

Graphoanalytical and statistical screening of data was used to exclude improbable data values, such as input mistakes, incorrect measurement units and wrong well identification numbers. Altogether, the data from 182 wells was used in this study. All wells were clustered in 29 different groups, but 3 groups were discarded due to data inconsistency. In each group there was at least one well with observed groundwater level time series data, representing the reference period. In the groups with more than one well, the observed groundwater level time series were transformed into normalized values and compared between each other, while wells with the worst data series and poor reciprocal correlation, were identified and discarded. The remaining observations were averaged over the group where they belonged. Clustered well group locations and the continentality index are represented in Fig.1.

Mathematical transformations

Interpolation was used to fill the daily values of missing observations. Studying correlations between groundwater level fluctuations and continentality in this research, it is crucial to minimize the influence of non-climatic parameters such as groundwater depth and the hydraulic properties of the aquifer medium. Standardization was done to remove the impact of local conditions such as different amplitude and absolute mean groundwater level, ground surface, slope, soil grading composition, land use, etc.

After the mathematical transformations the final data consists of three datasets. The first dataset represents observations in the reference period, the second – modelled groundwater levels in the reference period for each projection and the third – modelled groundwater levels in the future period for each projection. All datasets contain 12 standardized long-term monthly mean values for each clustered well group, with 312 values per dataset per projection altogether.

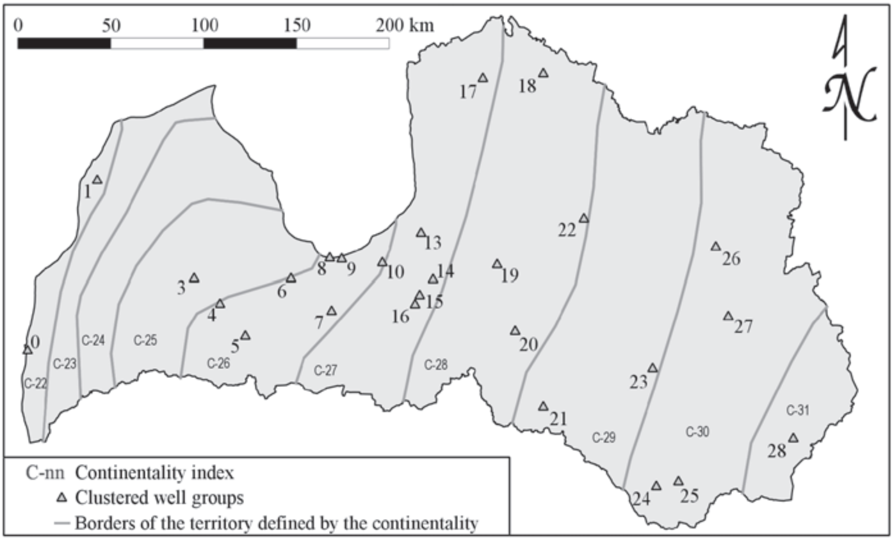

Figure 1. Geographically weighted centres of the clustered well groups (triangles) and the continentality index (isolines). Clusters No. 2, 11 and 12 were rejected and not shown in this figure.

Interpolation

There is a large variability in groundwater level monitoring frequency. Mostly groundwater level measurements are made every three days, but in the raw observed time series there are periods when the frequency was only once per week. The periods with monitoring frequency worse than 7 days were rejected. Otherwise, the interpolation (see equation (1)) of monitoring data was used in order to get the daily groundwater levels in each selected well. Such a statistical approach allows the equal weight the groundwater levels temporary.

$$l_i = l_{prev} - \frac{l_{prev} - l_{next}}{n} i \qquad (1)$$

In the equation (1): n is number of days between the previous and next observed groundwater levels, l_{prev} is the previous or the first measured groundwater level, l_{next} is the next or the last measured groundwater level, l_i - is the groundwater level in the i–th day, i is the number of day.

Standardization

The groundwater levels in the database are measured as a distance from the ground surface to the water table i.e. a larger value represents deeper groundwater.

In order to standardize groundwater data from different wells, time series containing mean monthly groundwater levels were normalized twice.

First, the groundwater observation series were inversely normalized for each hydrological year (12 month period starting from October) thus giving values between 0 and 1 using equation (2)

$$l_i^n = 1 - \frac{l_i - l_{\min}}{l_{\max} - l_{\min}} \quad (2)$$

Here l_i^n is the inverse normalized relative position of the groundwater table for the i–th month.; l_i is the absolute mean monthly groundwater level in the i–th month; l_{min} is the maximum mean monthly distance to groundwater level; l_{max} - is the minimum mean monthly distance to groundwater level.

After such a normalization approach, value 0 represents the deepest groundwater table level and value 1 represents the most shallow groundwater table level for each hydrological year. This transformation gives a more logical perception of groundwater levels – when groundwater has reached its minimum level, the value of l^n is 0, and when it reaches its maximum, the value of l^n is 1. Otherwise, after normalization the results can be easily misinterpreted, and, in transforming absolute to normalized groundwater levels, the latter was inversed subtracting the calculated value from the maximal possible value 1. In this study it is called first-time, inverse normalization. Using normalized data for each hydrological year, the long-term normalized mean groundwater levels were averaged for each month.

Second, normalization was made for the already normalized long-term monthly mean groundwater level l^n. The second normalization is a simple amplitude normalization calculation. The applied normalization method was adapted and modified from (Chelmicki, 1993).

$$l_i^N = \frac{l_i^n - l_{\min}^n}{l_{\max}^n - l_{\min}^n} \quad (3)$$

In the equation (3): l_i^n is the double normalized relative position of the groundwater table for the i-th month; l_i^n is the relative mean monthly groundwater level in the i-th month; l_{max}^n is the maximum mean monthly groundwater level; l_{mix}^n is the minimum mean monthly groundwater level.

Characterizing future climate projections by percentiles

Eleven members of the ensemble of future climate projections from the EU ENSEMBLES project (ENSEMBLES, 2009) were used for characterizing the future climate period 2071-2100. The ENSEMBLES data used in this work was funded by the EU FP6 Integrated Project ENSEMBLES (Contract number 505539). The regional climate models were further statistically downscaled removing systematic biases according to an approach by (Sennikovs and Bethers, 2009, Bethers et al., 2012). Each ensemble member has its own properties and specific characteristics which make it unique and together these climate projections create a model ensemble. One of the ways to describe such a model ensemble, including multiple data series, is to use percentiles. A percentile is the value of a variable below which a certain percent of calculated data fall. The values between the 17th and 83rd percentiles describe where most of the population – in our case – long term monthly mean groundwater level values projected by all ensemble members lie. There is no defined value for which percentiles limit and characterize multiple data. Describing multiple data series together some researchers use a median which is the 50th percentile (Nestler and Long, 1994), others – the 25th and 75th percentiles or quartiles (Haggard et al., 2005). When the data corresponds to a normal distribution, the values of these percentiles are very close to doubled sigma values. 66% or two thirds of the model ensemble are covered when the 17th and 83rd percentiles are used to describe a multiple data series.

Modelling

The METUL groundwater model is a mathematical conceptual hydrological model which calculates daily groundwater level (Krams and Ziverts, 1993). Model input data includes the daily mean air temperature, total amount of precipitation and vapour pressure deficit. In the previous study (Lauva et al., 2011), the modification of the model was done adding the user interface and the possibility of automatically calibrating parameters using a Simplex algorithm. Before the modifications, the calibration was done manually and input and calculated data management was rather uncomfortable. After the modifications the model was successfully used in other studies (Veinbergs et al., 2012).

Model parameters for each chosen groundwater level observation well were estimated by calibrating and validating the model on the observed groundwater levels in the reference period in the previous study (Lauva et al., 2012). Obtained parameters describe the hydrophysical properties of the chosen well and its surroundings. Assuming that these parameters do not considerably change over time, it is possible to compare model results, which are calculated in different time periods. In this study the model parameters previously obtained in the reference period were used to calculate the groundwater levels for the future time period with the METUL model. After the groundwater time series were calculated, a standardization (see above) was made for each well.

Mapping

Finally, mapping was done over all of Latvia using the geographical information system (GIS) Grass GIS (Grass GIS). It is open source software and has previously been widely used in a broad range of different geographical studies, such as groundwater flow calculation (Gebbert, 2007), land-use impacts on watershed response (Doe et al., 1996), drain network analysis (Jasiewicz, 2009), etc.

Relative long-term monthly mean values were interpolated using an inverse distance weighting interpolation method and the mapset was created for each percentile calculation. Each mapset contains 12 raster maps, which represent the spatial distribution of standardized long-term mean monthly groundwater levels. The raster statistics were calculated for all individual territories distinguished by continentality.

The described methods were borrowed, modified and enhanced for our study specifics from similar research done in Poland (Chelmicki, 1993).

Results and discussion

The results represent modelled relative long-term mean monthly groundwater levels for the reference climate period and 11 climate change projections for the future period. The results were analyzed by the degree of continentality and for the whole territory of Latvia.

Reference period

The previous results (Lauva et al., 2012) showed that in the reference period observed monthly mean, minimal and maximal annual cycles (Fig. 2.b) correspond to the groundwater regime in Latvia defined in (Толстов, 1986) - representing all four crucial groundwater regime extremes – autumn and spring maximums and winter and summer minimums. The same conclusion can be stated analyzing reference period results according to the degree of continentality (Fig. 2.a). See Fig. 1 for the spatial distribution of the continentality index.

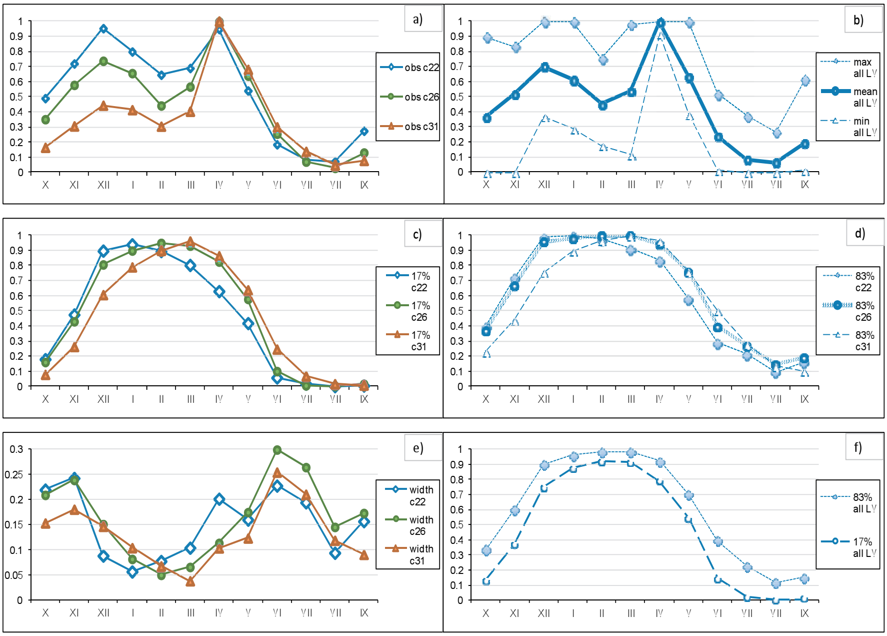

Figure 2. Monthly normalized groundwater levels (a) observations in the reference period (1961-1990) for three different continentalities, (b) observations in the reference period overall throughout Latvia, (c) 17th percentiles of the model ensemble for three different continentalities, (d) 83th percentiles for three different continentalities, (e) groundwater level difference between the 17th and 83rd percentile for three different continentalities, (f) 83% and 17% percentiles averaged over the whole of Latvia.

Future period

In the previous study (Lauva et al., 2012), using only one climate change projection, we concluded that (1) in the territories with a degree of continentality greater than 24, the groundwater seasonal regime will remain the same classical Latvian M-shaped groundwater level regime while (2) the winter groundwater level minimum will disappear for continentality indices below 24. These results can be explained by a different temperature regime which has an impact on snow accumulation during winter. For the lower C the winter thaws occur more frequently and subsequently the groundwater recharge in the winter period is increased.

The modelled results of the seasonal cycle of normalized groundwater levels for the ensemble of future climate projections are shown in Fig. 2c-2e. Analyzing the 17th percentile, the winter maximum differences between continentalities are clearly seen. Winter maximum occurs later in the territories with a higher continentality index. The minimum tends to be reached in June and it is prolonged till September (Fig. 2.c).

Analyzing the 83rd percentile border, the differences between different continentality indexes are also clearly seen. The character of the time shift for the winter groundwater level is the same as for the17th percentile (Fig. 2.d). In the autumn, groundwater levels increase more rapidly in territories with a lower continentality index, reaching a maximum already in December. A more gradual and not so steep increase occurs in the territories with a lower continentality index, reaching a maximum only in March.

Let us define the uncertainty of the groundwater monthly level as a difference between the chosen percentiles. These percentile values averaged over the set of wells (i.e. for the territory of the whole of Latvia) are shown in Fig.2.f . A larger difference means larger uncertainty in the groundwater level in that particular month. The largest uncertainty in groundwater levels is in the summer months June and July in all the territory – independent of continentality (Fig.2.e). The lower uncertainties are in the months when the winter maximum is reached for all continentality indices. The lowest uncertainty is in the winter maximum (March) and the largest continentality index (C=31). This can be explained by similarities between the members of the ensemble of climate projections affecting the groundwater regime.

The highest uncertainty is in the territories with a transitional continentality index (23-28) and that can be explained by different spatial shifting of the continentality index by different members of the climate projections ensemble (Fig. 2.e). Note that all climate change projections tend (1) to decrease the continentality index in comparison with the contemporary climate and (2) reduce the difference in the continentality index over the territory of Latvia (Bethers et al., 2012).

Distributions of spatial distribution of ground water level uncertainty during April and during December for the future period 2071-2100 are represented in Fig. 3. The clear impact of continentality on groundwater levels can be seen although uncertainty remains quite stable over all of the territory of Latvia.

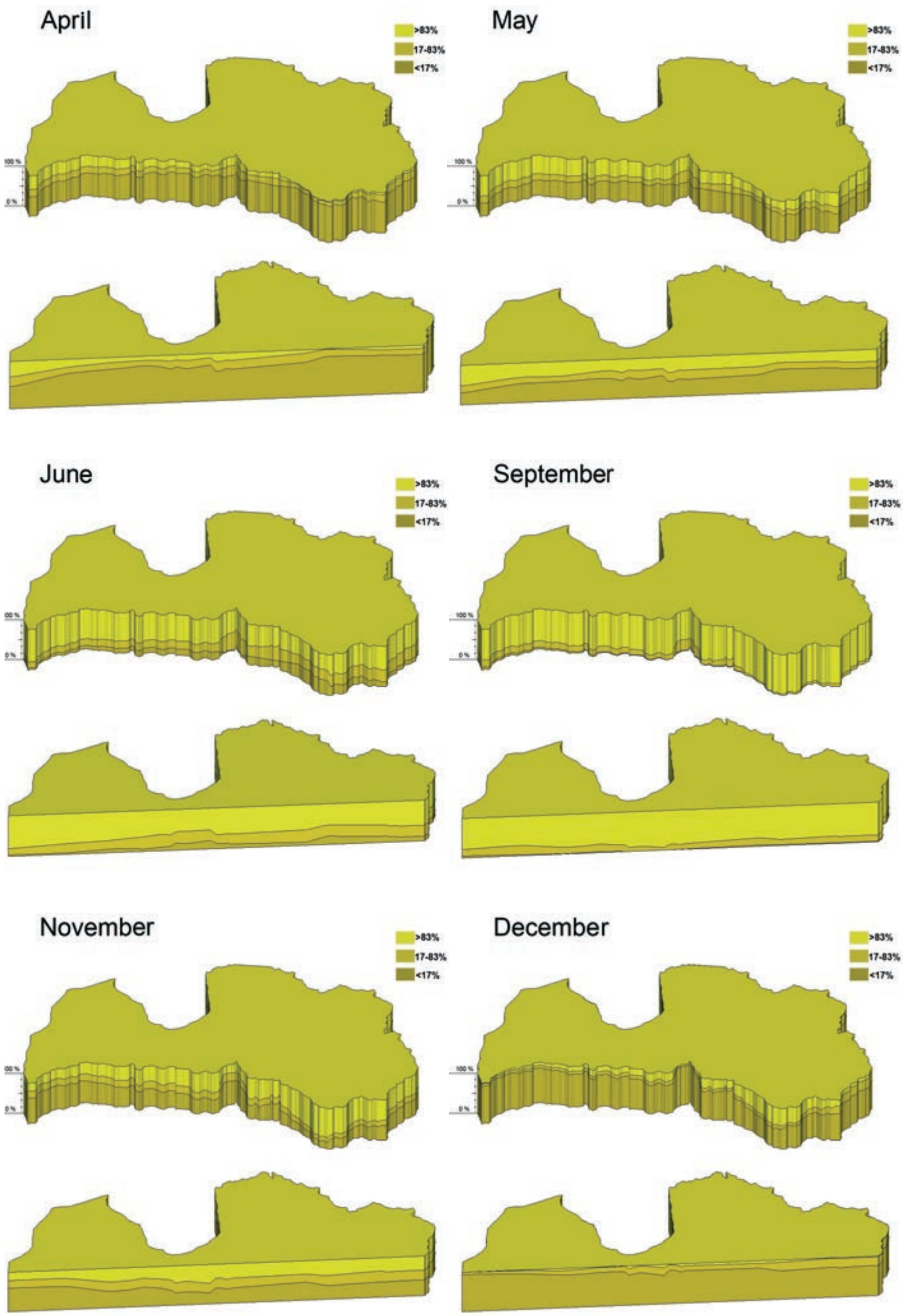

Figure 3. The 83% and 17% percentiles of the groundwater level for the future period (2071-2100) calculated from ensemble of 11 climate change projections over the whole of Latvia.

Conclusion

The main conclusions that can be drawn from the presented results are as follows:

1. In the reference period (1961-1990) both the observed and modelled monthly mean, minimal and maximal relative groundwater levels over the whole of Latvia correspond to the M-shaped classical groundwater regime in Latvia (Толстов, 1986) representing all four crucial relative long-term mean monthly groundwater regime extremes – winter and summer minimums and spring and autumn maximums.
2. This conclusion holds true for particular continentality index zones as well as for the spatially averaged data (over the territory of Latvia).
3. Uncertainty of the modelled ground water levels for the future period (2071-2100) exist within the ensemble of 11 climate change projections. One can clearly notice the transformation from an M-shaped to a Λ-shaped ground water seasonal cycle (regime).
4. The study proves that the METUL groundwater model is applicable to the groundwater level fluctuation studies and the model results are comparable with observations made during the reference period. Future research work on ground level variability may be focused on uncertainty assessment in the METUL model using Monte-Carlo or other methods.

It is possible to continue the research in a number of directions, for example, in obtaining the absolute groundwater levels spatiotemporally.

Acknowledgements

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Surface water-groundwater interactions in agricultural areas

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Abstract

To establish an empirical link between surface water and groundwater, a multiscale monitoring approach was proposed. A network of agricultural runoff monitoring stations was set up for long term observations of water quality and run-off from agricultural areas by Latvia University of Agriculture (LLU). This included measurements at three different monitoring scales, i.e. drainage field, small catchment and groundwater. The long-term (1995 - 2011) water quality, runoff and groundwater level measurements from three monitoring stations (Bērze, Mellupīte and Auce) and three additional groundwater monitoring points (Staļģene, Oglaine and Miltiņi) showed large variations in nutrient concentrations depending on the research scale. In terms of water quality, the highest nitrogen and phosphorus concentrations were recognised in the drainage field, but the lowest concentrations were in the groundwater scale. However, water quality in the small catchment was closer to the determined values in the drainage field scale. It is evident that runoff from the small catchment (agricultural areas with drainage systems) is mainly formed by subsurface tile drainage runoff. The results also proved the strong correlation between average depth where the water quality (N_{tot} and P_{tot}) forms from within all the scales. In general, the water quality is better in the groundwater wells as it is formed in greater depth.

Keywords: agriculture; water quality; monitoring scales

Introduction

Water resource quality and availability is a worldwide problem and a research field in many countries. Currently, the impact of agriculture on water ecosystems is being frequently discussed for scientific, economic and political reasons. The emmision of nutrients (nitrogen and phosphorus) from different economic activities can cause extreme contamination of water bodies. The enrichment of nutrients in a water environment starts a eutrophication process and changes an ecosystem's stability. Nutrient emissions from agricultural activities can reach water bodies - lakes, rivers, streams and seas.

The nitrogen cycle is mainly based on biogeochemical processes by whitch nitrogen transforms into solid, liquid or gaseous form and moves through air, soil, water and living organisms. Nitrogen is required for all organisms to live and grow as it is a constitution of the deoxyribonucleic and ribonucleic acids, as well as protein. The main nitrogen transformation processes performed by microorganisms are fixation, plant/animal uptake, mineralization, nitrification and denitrification.

The human influences on the phosphorous cycle come mainly from the application of fertilizers in agricultural ecosystems. For example, animal wastes and manure being applied to farmland as fertilizer. Plants are not always able to utilize all of the phosphate fertilizer applied, and as a consequence, much of it is lost from the soil surface layers through water run-off.

Nitrogen and phosphorus are major key elements for plant growth, especially, in agricultural ecosystems. The availability of different nitrogen and phosphorus compounds are of the utmost importance for crop capacity (Gustafson et al., 1997).

Agricultural activity has resulted in the application of fertilizer and can always be expected to contribute nutrient loading in surface waters, drainage runoff and groundwater as a diffuse source. Fertilization has a long term effect on the nutrient availability for plants, moreover for water quality. Accumulation of N and P will occur through the soil profile and can be removed from the soil with microbiological and chemical processes in the soil environment and through harvesting. The leaching of nutrients to water bodies is an environmental aspect from the use of chemicals in agriculture (Regulations of the Cabinet of Ministers No 33). The enrichment of water bodies with nutrients is acknowledged as a major problem in many European countries.

Many studies focus on surface water quantity and its interactions with drainage runoff (Jansons and Butina, 1998) and groundwater (Rudzianskaité, 2006). The intensity and duration of discharge from agricultural areas mostly depend on meteorological and hydrological conditions. The identification of hydrological conditions in the mentioned areas is described as water discharge measurements in different scales. Water measurements and sampling were carried out in three different levels in small catchment, drainage field and groundwater. The main parameters analyzed and described in this study are total N (N_{tot}) and total P (P_{tot}). The interaction between discharge measurements and nitrate and phosphorus leaching are of major importance for this study.

Materials and methods

Agricultural runoff monitoring in Latvia was established in 1993 within the Baltic Sea Regional Programme (BSRP) and was provided by Latvia University of Agriculture. The agricultural runoff monitoring stations Bērze, Auce, Mellupīte and the groundwater monitoring points Staļģene, Oglaine, Miltiņi are located in diverse parts of Latvia and represent regions with a different climate, soil, crops and farming intensity. The sampling strategy was elaborated in accordance with the Water Framework Directive (EEC, 2000) and the Nitrate Directive (EEC, 2006). Water samples for hydrochemical analyses (N_{tot}, P_{tot}) of the small catchment and drainage field were taken on a monthly basis, but the groundwater samples were taken four times per year within each season (autumn, winter, spring and summer).

Water discharge measurements in open channel (small catchment) and tile drainage were quantified at a measuring station using Crump and triangular weir (V notch), respectively, but the groundwater table was measured by submerged water level sensors in observation wells. The processes at three monitoring stations (Fig. 1) have been examined by investigating the available monitoring data since 1995 – 2011. Additional shallow groundwater monitoring points (Staļģene, Oglaine and Miltiņi from 2011) were set up in vulnerable areas to monitor diffuse and point source pollution from agricultural activities.

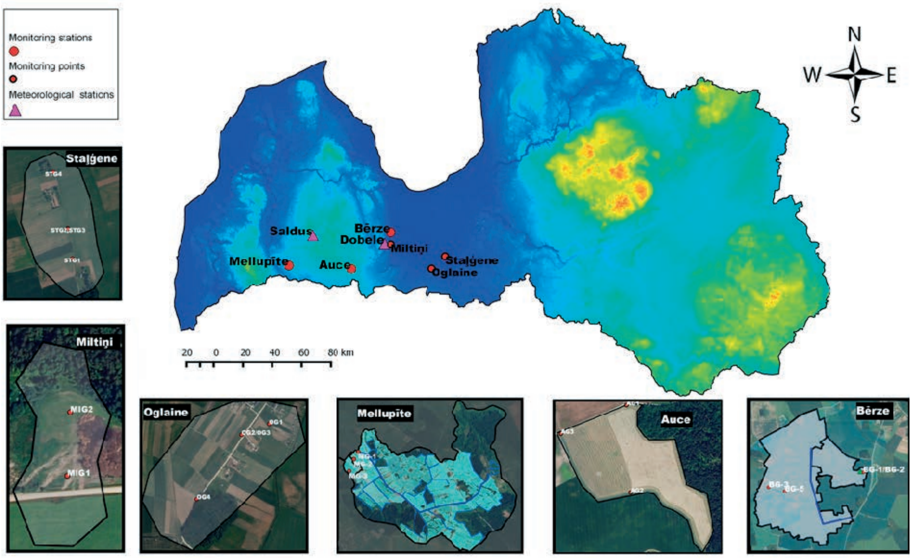

Figure 1. The LLU monitoring stations, points and (LEGMC) meteorological stations.

Site description

Groundwater monitoring in agricultural territories was set up for agricultural impact assessment on groundwater quality. The screen interval of observation wells for groundwater sampling is from 2 to 6 m in depth (Tab. 1). Each observation well is equipped with data loggers to obtain hourly average groundwater levels.

Table 1. Characteristics of observation wells at monitoring sites.

Monitoring site	Bērze				Mellupīte			Auce				Miltiņi		Staļģene				Oglaine			
Observation well	BG-1	BG-2	BG-3	BG-5	MG-1	MG-2	MG-3	AG-1	AG-2	AG-3	AG-4	MIG-1	MIG-2	STG-1	STG-2	STG-3	STG-4	OG-1	OG-2	OG-3	OG-4
Depth of observation well	23	5.7	8	5.2	7	4.5	11	6	6	10	5.4	10	11	6	5	18	6	7	6.5	12	8
Screen interval from - to, m	13.0 - 17.0	2.0 - 6.0	4.0 - 7.7	2.0 - 4.8	2.0 - 6.7	2.0 - 4.2	6.0 - 10.7	2.0 - 5.7	2.0 - 5.7	4.0 - 8.0	1.8 - 4.6	1.75 - 3.75	1.8 - 3.8	2.8 - 4.8	2.65 - 4.65	12.9 - 17.9	2.85 - 4.85	3.65 - 5.65	2.6 - 4.6	6.9 - 11.9	3.65 - 5.65
Soil description	Silt loam				Clay loam			Sandy loam				Loamy till		Alluvial and limnoglacial sand				Loamy till interbedded by sand and gravel			

The **Bērze** agricultural runoff monitoring station (small catchment 368 ha, drainage field 76.6 ha) (Fig. 1) is located in the Dobele District, Jaunbērze Parish. The thickness of quaternary deposits is 10 – 20 m. Calcic Cambisol according to FAO classification (1990) is the dominating soil type at Bērze monitoring station. The composition of the top soil is as follows: 10.5% clay, 54.96% silt and 34.54% sand. Four observation wells (BG-1, BG-2, BG-3 and BG-5) have been constructed at the monitoring station (Tab. 1). Runoff measurements for catchment and drainage research were started in 1968 both in the main catchment and from a composite field drainage system adjacent to the main catchment. At catchment discharge was measured by a modified Crump flat-V weir, but drainage discharges were measured using a V-notch weir. Average hourly water levels were recorded in data loggers for discharge measurements.

The **Mellupīte** agricultural runoff monitoring station (small catchment 960 ha, drainage field 12.9 ha) is located in the Saldus District (Fig. 1), Parish Zaņa. The thickness of quaternary deposits is 10 – 20 m. According to the soil texture, the dominant soil is clay loam. Most of the agricultural area is drained with tile drains (depth 1.1 – 1.3 m, spacing between drains 10 – 32 m) (Vagstad et al., 2001). The composition of the top soil is 11.9% clay, 40.95% silt and 47.15% sand. Three observation wells (MG-1, MG-2, and MG-3) were constructed at the monitoring site in 2005 (Tab. 1). Measurements were carried out at all three scales: catchment, drainage field and groundwater. At the main catchment, a Crump weir was used for discharge measurements while a V-notch was used at the drainage field. Average hourly water levels were recorded in data loggers for discharge measurements.

The **Auce** agricultural runoff monitoring station (small catchment 60 ha, drainage field 60 ha) (Fig. 1) is located in the Auce District, Vecauce Parish. The moraine landscape, created by the last glaciations, has produced naturally fertile soils at the Auce monitoring station. The thickness of the quaternary sediment layer is 10 – 30 m. The dominant soil according to the soil texture of the moraine is sandy loam (Vagstad et al., 2001). Most of the agricultural areas at the Auce monitoring station are drained with tile drains (depth 1.1 – 1.3 m) (Vagstad et al., 2001). The textural composition of the top soil is 2.35% clay, 34.35% silt and 63.30% sand. Four observation wells (AG-1, AG-2, AG-3 and AG-4) were constructed at the monitoring station (Tab. 1). Runoff changes over the period were estimated by hydrological modelling results.

The **Staļģene** monitoring point (Fig. 1) is located in the Jelgava District, Jaunsvirlauka Parish. The monitoring point was established on Lielupe alluvial plain and the thickness of quaternary deposits varied from 2.5 – 7.0 m. Groundwater depth in the area is from 0.7 – 1.5 m below the soil surface. The quaternary deposits at Staļģene monitoring point in the upper part of the profile consist of alluvial and limnoglacial sand, but in the lower part, loamy till. The quaternary deposits are underlayed by upper Devonian clays with sandstone streaks (Joniškį formation). Four observation wells (STG-1, STG-2, STG-3 and STG4) were constructed at the monitoring point (Tab. 1).

The **Oglaine** monitoring point (Fig. 1) is located in the Jelgava District, Vircavas Parish. The thickness of the quaternary deposits varied from 5.0 – 7.0 m. The groundwater depth in the area is from 0.4 – 1.2 m below the soil surface. The quaternary deposits at the Oglaine monitoring point consist of loamy till interbedded by sand and gravel. The quaternary deposits are underlayed by upper Devonian dolomitic sandstone with clay streaks (Kursa and Joniškį formation). Four observation wells (OG-1, OG-2, OG-3 and OG-4) were constructed at the monitoring point (Tab.1).

The **Miltiņi** monitoring point (Fig.1.) is located in the Dobele District, Bērze Parish. The thickness of the quaternary deposits varied from 14.0 – 17.0 m. The groundwater table depth in the area is from 0.1 – 0.9 m below the soil surface. The quaternary deposits at Miltiņi monitoring point consist of loamy till (Weichselian glaciations). The quaternary deposits are underlayed by upper Devonian dolomites (Joniškį formation). Two observation wells (MIG-1 and MIG-2) were constructed (Tab. 1).

Table 2. Observations at LLU monitoring stations.

Monitoring station, parameters		2000	2001	2002	2003	2004	2005	2006	2007	2008	2009	2010	Average
Bērze	Amount of precipitation, mm	507	713	677	469	618	515	487	565	531	574	827	589
	Small catchment runoff, mm	130	230	190	121	175	163	40	80	108	111	306	150
	Drainage field runoff, mm	128	171	108	57	175	93	61	163	169	135	332	145
	BG-1, groundwater depth, cm	-	-	-	-	-	-	43	1	24	-4	-56	2
	BG-2, groundwater depth, cm	145*	125*	133*	194*	146*	159*	207	149	152	151	123	153
	BG-3, groundwater depth, cm	79*	58*	81*	146*	91*	94*	130	80	89	80	61	90
Mellupīte	Amount of precipitation, mm	597	773	595	586	604	473	579	757	650	862	855	666
	Small catchment runoff, mm	153	243	288	130	229	150	168	242	184	256	361	219
	Drainage field runoff, mm	174	246	270	137	180	147	198	303	218	285	372	230
	MG-1, groundwater depth, cm	170*	148*	164*	203*	161*	154*	133	128	128	115	119	148
	MG-2, groundwater depth, cm	242*	207*	230*	246*	213*	236*	221	179	195	162	170	209
	MG-3, groundwater depth, cm	366*	333*	350*	366*	337*	363*	344	291	323	305	295	334
Auce	Amount of precipitation, mm	507	712	670	469	651	582	613	758	650	862	-	686
	Runoff, mm	184	469	315	167	482	367	439	643	589	757	-	456
	AG-1, groundwater depth, cm	137*	125*	129*	142*	123*	133*	98	70	78	66	60	74
	AG-2, groundwater depth, cm	191*	182*	191*	191*	184*	187*	146	139	146	133	129	139
	AG-3, groundwater depth, cm	41*	26*	46*	43*	29*	38*	46	4	5	53	272	76
	AG-4, Groundwater depth, cm	82*	68*	68*	88*	72*	71*	85*	56*	72*	37	35	36

Note (*) modelled groundwater depth with METUL (Krams and Zīverts 1993).

Meteorological station data (precipitation, temperature, vapour pressure deficit) provided by the Latvian Environment, Geology and Meteorology Centre LEGMC were used for the modelling of groundwater levels (Tab. 2). Meteorological data were measured at the nearest Saldus and Dobele meteorological stations (Fig. 1). The meteorological data from Dobele station was used for Bērze monitoring station, but data from the Saldus meteorological station for Auce and Mellupīte monitoring stations.

Results and discussion

The water quality at the monitoring sites was assessed by presenting a N_{tot} and P_{tot} data comparison between monitoring sites (Fig. 2 and Fig. 3). The results of the obtained water quality data show that the highest variation of nitrogen concentrations (Fig. 2) were in the drainage field scale (0.6 - 102 mgL^{-1}) compared to the small catchments (0.53-29.5 mgL^{-1}) and groundwater research scale (0.15 – 26.4 mgL^{-1}). A similar trend was also observed for phosphorus (Fig. 3), i.e., the highest variation of P_{tot} concentrations was for the drainage field scale (0.003–5.30 mgL^{-1}) then in the small catchment scale (0.004–2.13 mgL^{-1}) and the groundwater observation wells (0.001-0.38 mgL^{-1}).

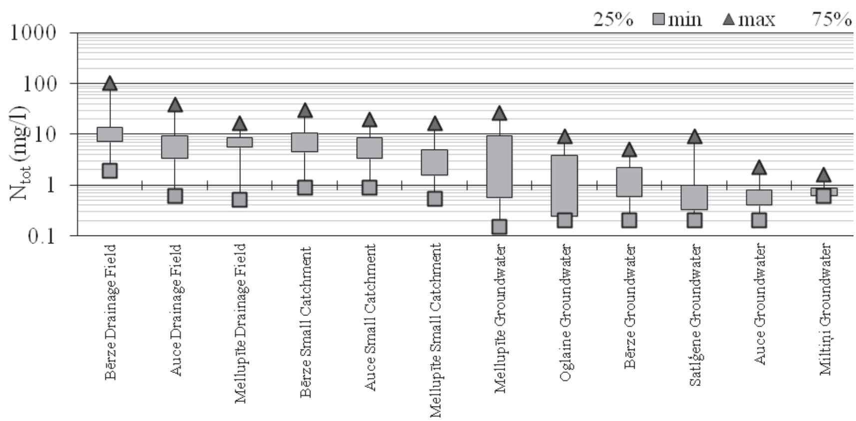

Figure 2. N_{tot} concentrations mgL^{-1} at LLU monitoring sites.

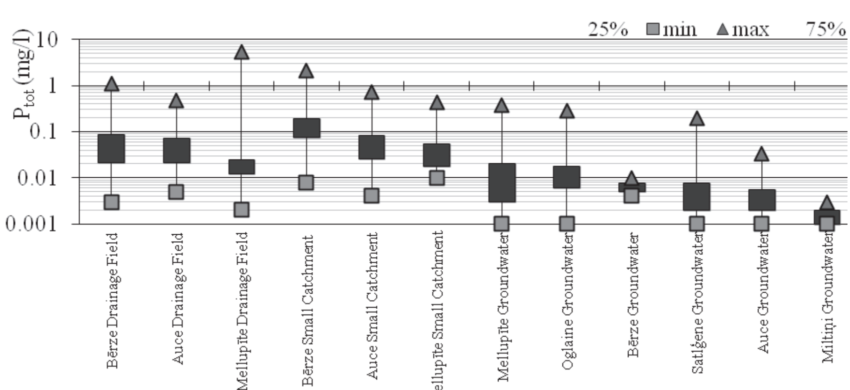

Figure 3. P_{tot} concentrations mgL^{-1} at LLU monitoring sites.

In general, a similar trend was also observed for phosphorus (Fig. 3). The highest variation of P_{tot} concentrations were for the drainage field scale (0.003–5.30 mgL^{1}) then in the small catchment scale (0.004–2.13 mgL^{-1}) and the groundwater observation wells (0.001-0.38 mgL^{-1}). However, the general data set of 25-75 percentiles shows that there are higher phosphorus concentrations in the small catchment scale and this could be explained by phosphorus immobility through the soil profile and increased transportation with surface runoff. Therefore, groundwater quality is less vulnerable to phosphorus leaching compared to nitrogen. The groundwater scale allows for the determination of the interaction between groundwater depth and water quality changes. For example, runoff with dissolved nitrate ions (NO_3^-) in different monitoring scales is formed in soil affected by groundwater. The NO_3^- is transported by groundwater flow (Canter, 1996). In different monitoring scales the dominant flow forms at a different depth (Fig. 4): in groundwater wells C; in drainage field B; in small catchment D.

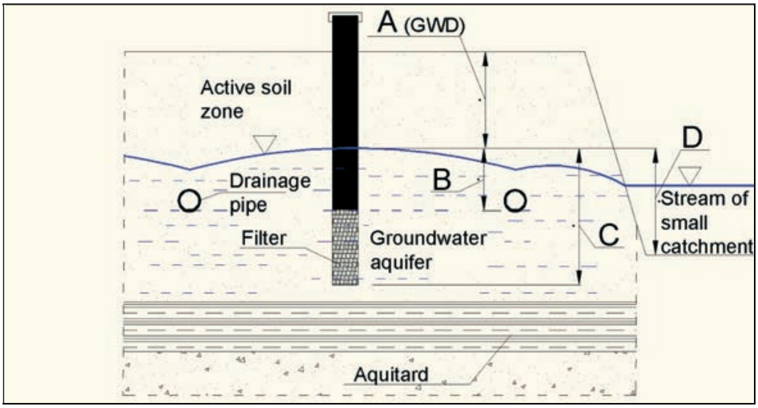

Figure. 4. Dominant groundwater flow in different monitoring scales.

The runoff from soil to open streams (small catchment scale) is formed by base flow and subsurface drainage runoff (Fig. 4). In the period of subsurface drainage runoff, frequently the main part of the total runoff is formed by subsurface drainage water. The base flow could be very low in comparison. The described situation is characteristic in heavy soils with a relatively thin layer D (Fig. 4). Consequently, the depth from where the dominant flow forms is decreased because of relatively high subsurface drainage runoff intensity. It should be mentioned that drainage runoff occurs if the groundwater is high enough to form a pressure higher than the hydraulic resistance of tile drainage and soil (Krams and Zīverts, 1993).

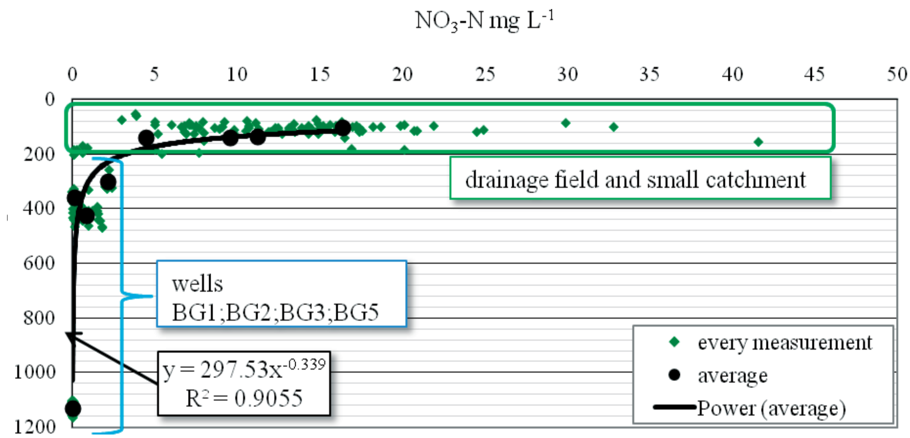

Figure 5. N-NO_3^- concentrations in runoff from different deptsh of groundwater at Bērze.

In the analysis of groundwater fluctuation impact on NO_3^- concentrations in the small catchment, it is very important to take in account the situation previously stated. There is an investigation of agricultural runoff at Bērze monitoring station (Fig. 5).

Nitrate nitrogen (N-NO_3^-) concentrations in three monitoring scales (groundwater scale, drainage field and small catchment) were studied, considering the impact of groundwater depth (GWD). The results demonstrate that there is less N-NO_3^- concentration in deep groundwater than is stated in a drainage field characterized by runoff from shallower groundwater. Also the runoff from the small catchment forms from a very similar depth if the subsurface drainage becomes dominant. The impact of groundwater fluctuations on N-NO_3^- concentrations in both drainage runoff and runoff from the small catchment is comparatively high – the gradient for nitrate nitrogen concentration against an increase of groundwater depth by 1 cm (N-NO_3^-/GWD) is 0.34...0.38 (mgL^{-1})/cm. In the groundwater scale the gradient is 0.001...0.038 (mgL^{1})/cm.

The changes in groundwater fluctuation seasonally could affect the leaching of the nitrogen accumulation process. The forward studies should be based on combining future climate impact on groundwater quality using different modelling techniques. Agricultural runoff monitoring provided by LLU in different scales (small catchment, drainage field and groundwater) is required to evaluate agricultural impact on water bodies and to promote scientific conclusions and recommendations in future.

Conclusions

The highest variation of nitrogen concentrations (Fig. 2) is in the drainage field scale (0.6 - 102 mgL^{-1}) compared to the small catchments (0.53-29.5 mgL^{-1}) and the groundwater research scale (0.15 – 26.4 mgL^{-1}).

The highest variation of P_{tot} concentrations is for the drainage field scale (0.003–5.30 mgL^{-1}) then in the small catchment scale (0.004–2.13 mgL^{-1}) and the groundwater observation wells (0.001-0.38 mgL^{-1}).

Groundwater quality is less vulnerable to phosphorus leaching than to nitrogen.

In the small catchment level the closer the groundwater table is to earth surface the higher is the risk of N-NO_3^- leaching potential. It leads to higher concentrations.

In those small catchment streams where the base flow is dominant, better water quality could be expected.

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