NUMERICAL SIMULATION OF GROUNDWATER FLOW AND HEAT TRANSPORT OVER GEOLOGICAL TIME SCALES AT THE MARGIN OF UNCONFINED AND CONFINED CARBONATE SEQUENCES

PhD thesis

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“Simplicity is not about deprivation. 
Simplicity is about a greater appreciation for things that really matter.”

Anonymous
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1 INTRODUCTION

1.1 Background and objectives

It has been recognised for decades that the occurrence and movement of groundwater affects a wide range of geologic processes (Bredehoeft and Norton, 1990; Garven, 1995). Due to its interactions with the ambient environment and its spatial distribution, groundwater flow can mobilize, transport and deposit matter and heat, lubricate discontinuity surfaces in the rock framework as well as generate and modify pore pressures (Tóth, 1999). Improved knowledge of flow system hydrodynamics is thus required to better understand its role in affecting geologic processes.

Groundwater flow systems are also not static, flow mechanisms evolve continuously during the geological history of their host basins (Ingebritsen et al., 2006). Transient hydraulic and thermal conditions could therefore evolve, for example, in response to a variety of changes including those related to tectonic uplift and stress, sediment compaction, erosion, thermal conditions, geochemical reactions or climate (Deming, 2002).

As Fowler and Grasby (2006) showed, the often-implied presumption that present-day hydrodynamics of a basin can be used to interpret past fluid migration events is likely to be false due to re-oriented flow paths caused by changing geological conditions. Therefore, understanding the transient history of subsurface fluid flow systems could be essential and would help to explain the role of groundwater in a number of geologic processes from crustal heat transfer, diagenesis, metamorphism, formation of evaporates, hydrothermal flow and ore genesis, hydrocarbon migration and porosity enhancement to hypogene karstification (Bredehoeft and Norton, 1990; Garven, 1995; Goldscheider et al., 2010; Ingebritsen and Sanford, 1999).

In the case of deep carbonate systems (more than 3000 m deep, Alley et al., 2013), the significance of changes in flow patterns and heat distribution over long time scales lies in its effects on the development of permeability and accumulation of heat, which e.g. can help to identify the geothermal and hydrocarbon resource potential of deep carbonate systems as well as prospective areas for carbon dioxide sequestration (Goldscheider et al., 2010).

A particularly interesting flow pattern arises at the margin of confined and unconfined carbonate sequences as pointed out based on steady-state simulations for the analogue area of Buda Thermal Karst (BTK) by Mádl-Szőnyi and Tóth (2015). However, the complex transient evolution of the proposed flow pattern has not yet been investigated. In such locations, regional fluid migration pathways are likely to have varied considerably throughout the geological evolutionary period.
due to the topographical changes associated with vertical uplift and its consequences on gravity-driven groundwater flow. Therefore, these changes in conditions might have also had implications on mass and heat transfer.

In case of long geological time scales, numerical simulation methods are often the only feasible means of interpreting data and producing insight into the response of groundwater systems to transient processes acted in the past. Therefore, in the current study, semi-synthetic snapshot models of coupled density-dependent flow and heat transport were used to gain insight into the paleohydrogeology and thermal history of marginal areas of confined and unconfined carbonate sequences within the context of the Buda Thermal Karst (Hungary) as an analogue system. Based on these snapshot simulations, we can follow the effects of changing conditions on the fluid-potential and heat distribution during the geological evolution of the basin. The main goal of the study is to answer the following questions: i) What are the main characteristics of the flow field and temperature distribution in these marginal carbonate systems with decreasing cover thickness at one ridge?, ii) What are the main effects of low-permeability confining formations with changing thickness overlying a permeable carbonate system?, and iii) What is the relative importance of gravity and buoyancy as main driving forces in the different geological evolutionary stages with different confining layer thicknesses?

Effects of transient flow evolution on heat distribution, permeability, as well as groundwater geochemistry in deep confined and unconfined carbonate basins can then be interpreted in further studies based on these results and can provide a suitable background to clarify more detailed site-specific mass and heat transfer related questions.

1.2 Regional-scale groundwater flow in carbonate systems and approaches for its numerical interpretation

Several characteristics of carbonate systems make the numerical representation of its hydrogeological processes relatively difficult, especially in a highly karstified medium. Numerical challenges originate mainly from i) the continuous evolution of the aquifer due to dissolution (Goldscheider and Drew, 2007), ii) the large spatial heterogeneity and temporal variability of the system (Bakalowicz, 2005), iii) the scale effect of hydraulic conductivity (Király, 1975), iv) the duality of porosity, flow and storage (Király, 1998), as well as v) conduit networks with high flow velocity and turbulent flow (White, 2002).

It is well known that groundwater flow in sedimentary basins is organized into different orders of flow producing a nested system with local, intermediate and regional flow paths (Tóth, 1963), due to the particular distribution of the fluid potential (Hubbert, 1940). Although the gravity-
driven regional groundwater flow (GDRGF) concept was first developed for siliciclastic sedimentary basins, carbonates were more recently put into a basinal groundwater flow context. Klimchouk (2007) was the first to recognize that epigene karstification corresponds to local flow systems, while hypogene to regional or intermediate systems, and revealed the significance of hydraulic continuity proposed by Tóth (1995).

Based on the considerations of Mádl-Szőnyi and Tóth (2015), similar to siliciclastic basins, regional scale groundwater movement in thick carbonate regions has to be handled as cross-formational gravity-driven flow induced by fluid potential differences at the water table. They presented basic arguments supporting the applicability of the GDRGF concept in carbonates such as (i) the higher hydraulic diffusivity (D), (ii) the more efficient hydraulic connectivity and (iii) the scale dependence and wide range in hydraulic conductivity of carbonates:

(i) Hydraulic diffusivity is the ratio of hydraulic conductivity (K) and specific storage (S₃) of the given formation. Lithified carbonate rocks have lower specific storage (10⁻⁴ – 3×10⁻⁶ m⁻¹) compared to siliciclastic material (2×10⁻² – 10⁻⁴ m⁻¹) (Batu, 1998), while karst limestone, limestone and dolomite have higher hydraulic conductivity (2×10⁻² – 10⁻⁶ ms⁻¹, with a minimum value of 10⁻⁹ ms⁻¹) compared to the consolidated rocks of sedimentary basins (6×10⁻⁶ – 10⁻¹³ ms⁻¹) (Domenico and Schwartz, 1990).

(ii) Because hydraulic diffusivity is higher, hydraulic continuity is more effective in carbonate rocks compared to siliciclastic basins, i.e. hydraulic head changes propagate at higher velocities and over greater distances and depths in a carbonate rock framework (Klimchouk, 2009; Mádl-Szőnyi and Tóth, 2015).

(iii) Moreover, due to deep fractures and major faults and conduits, which can form preferred groundwater flow pathways, the mean hydraulic conductivity of a carbonate region increases with increasing control volumes. Even a four orders of magnitude increase could be present in K values derived from laboratory samples compared to those found in pumping tests, and another four orders of magnitude increase from water balance studies for an entire basin in karstified carbonates (Király, 1975).

However, in parallel, as the scale of the investigation increases, the variation of the effective hydraulic parameters of the system decreases (Figure 1). On small, local scales, the variations in porosity and hydraulic conductivity are very high, and turbulent flow takes place in the conduits. In contrast, on larger, regional scales, according to the representative elementary volume (Bachmat and Bear, 1987; Bear, 1972), the parameters could be considered as constant, and the flow system can be considered as representing an integrated ensemble of matrix, fracture and channel processes. As a consequence, local effects of karstic heterogeneities, such as karst
conduits, tend to average out over larger areas, and may be neglected on regional scale (Abusaada and Sauter, 2013; Wellman and Poeter, 2006).

Most of the karst-related distributive numerical modelling approaches try to represent the flow field better through the understanding of the effect of fractures and channels and their relations to the matrix (Dverstorp et al., 1992; Faulkner et al., 2009; Graf and Therrien, 2007). On the other hand, understanding the hierarchical patterns of gravity-driven regional groundwater flow in carbonate regions has not yet received much focus.

![Conceptualization of the representative elementary scale, showing where the parameters of a studied system could be considered as constant (after Bear, 1972)](image)

Consequently, the selection of an appropriate numerical simulation method depends on the given hydrogeological problem to be solved and questions to be answered. That is the selection depends primarily on the scale of the system, the degree of karstification, and data availability. Three main methods are available to describe flow in karstified carbonate systems, as outlined below.

(i) The combined discrete-continuum (CDC) approach models the matrix as a continuum in which the karst conduits are embedded as discrete elements (Király and Morel, 1976). In this way, the spatial influence of the karst conduits on groundwater levels in the matrix can be calculated throughout the karst system (Figure 2a).

(ii) The dual-continuum (DC) approach considers the heterogeneity of karst systems through the definition of two interacting continua, one for the matrix and another one for the karst conduits (Teutsch and Sauter, 1991). Both continua exchange water as a function of their water level, therefore it can describe the dual behaviour of karst aquifers (Figure 2b).

(iii) The equivalent porous medium (EPM) approach assumes that hydraulic heterogeneities can be represented by “average” properties within the validity range of representative
elementary scale (Teutsch and Sauter, 1991). On the local, aquifer scale, it is considered inappropriate because it overlooks the heterogeneity and anisotropy of the karst. However, it can be used on regional scales, since local influences of karst conduits may average out over larger areas (Lapcevic et al., 1999) (Figure 2c).

![Diagram of karstified carbonate system](image)

*Figure 2 – Representation of a karstified carbonate system by the main types of distributed modelling approaches. a) CDC – combined discrete-continuum approach, b) DC – dual-continuum approach, c) EPM – equivalent porous medium approach (after Hartmann et al., 2015)*

In general, dual-continuum and combined discrete-continuum approaches are appropriate on local scales for shallow karst systems – on which scale the coupling of matrix, fracture, and conduit flow is necessary to describe the entire karst system –, while the equivalent porous medium approach can be applied only for regional scale modelling of carbonate basins (Abusaada and Sauter, 2013; Mádl-Szőnyi and Tóth, 2015; Wellman and Poeter, 2006). Since the current study focuses on regional groundwater flow processes rather than on more detailed local predictions of flow directions or rates, an equivalent porous medium approach was applied.
2 Numerical Simulation Framework

The Buda Thermal Karst (BTK) system in Hungary is considered as a pilot area for numerical studies. Since the focus of the numerical investigation is on the effects of transient system evolution on regional-scale groundwater flow and heat distribution, detailed fully transient and site-specific geological evolution is considered less important for the numerical interpretation. The main hydrostratigraphic units and their changes within the framework of geological evolution within the pilot area were also taken into account. Based on this consideration, the overview of the pilot area also focuses on the main aspects of system evolution over the last 10 million years instead of the complete transient description of the geological evolution for the BTK.

Prior to the numerical flow and heat transport analysis, several issues were addressed to frame the development of a realistic conceptual model. (i) Dimensionality and required complexity of the model, (ii) configuration of the water table and (iii) the possible driving forces for groundwater flow.

2.1 Pilot area

The Buda Thermal Karst (BTK) is situated at the margin of unconfined and confined carbonate systems (Figure 3). The conceptual models, and framework of the numerical models, have been supported by extensive field studies which have provided insight into the current hydrogeological system (Alföldi et al., 1968; Erhardt et al., 2017; Erőss, 2010; Eröss et al., 2012a; Mádl-Szőnyi and Tóth, 2017; Papp, 1942), and have helped to understand the governing paleo-fluid migration processes (Erőss et al., 2008; Erőss et al., 2011a; Kovács and Müller, 1980; Mádl-Szőnyi et al., 2018; Mádl-Szőnyi et al., 2015; Poros, 2011; Poros et al., 2012; Scheuer and Schweitzer, 1980). This extensive knowledge about the geological, speleological and hydrogeological conditions of the BTK have provided a base for the numerical investigations (including validation of the results), and have helped to place the groundwater flow simulations into a realistic geological evolutionary context.

Geological evolution of the pilot area over the last 10 million years

The BTK is the north-eastern discharge zone of the Transdanubian Range (TR), in the central part of the Pannonian Basin. The Pannonian Basin was formed as an extensional back-arc basin during the late Early to Middle Miocene syn-rift phase (~18–11 Myr) and the subsequent post-rift phase (~11–6 Myr) of thermal subsidence (Fodor et al., 1999; Horváth and Royden, 1981; Royden and
Horváth, 1988; Tari et al., 1992). Due to the thinned lithosphere below the basin, the entire area was characterized by an elevated heat flux (an average of 120 mWm\(^{-2}\) below the BTK) during the Middle Miocene, which has gradually decreased to an average of 100 mWm\(^{-2}\) (below the BTK) by recent time (Balázs et al., 2017; Balázs et al., 2016; Lenkey et al., 2002).

Figure 3 – a) Location of the pilot area within the Pannonian Basin (edited after Horváth et al., 2006), and b) morphological catchment area of the Buda Thermal Karst (white dashed line, after Mádl-Szőnyi et al., 1999) with trace of the geological cross-section of the area used for numerical interpretation (Fodor, 2011) (see in Figure 6)
By the Late Miocene (~11 Myr), the basin was isolated from the Paratethys open-sea system and became a brackish-freshwater lake known as Lake Pannon. Infill of the basin began with a major delta system from the NW and NE towards the basin interior (Figure ) (Gábris and Nádor, 2007; Magyar et al., 1999; Magyar et al., 2013), since the sediment accumulation rate significantly exceeded the rate of slowing thermal subsidence (Jámbor, 1989; Magyar et al., 1999).

During regression of Lake Pannon, the area gradually became subaerially exposed (Figure 4). After about 10 Myr (early Late Miocene) development of the modern drainage pattern of the Pannonian Basin started with incision of the paleo-Danube (Gábris and Nádor, 2007; Magyar et al., 2013).

From the Late Miocene (~8 Myr), structural inversion of the Pannonian Basin began (Uhrin et al., 2009), which contributed to the uplift of certain blocks, including the TR (Bada et al., 2007; Bada et al., 1999; Cloetingh et al., 2006; Gerner et al., 1999; Horváth et al., 2006a; Horváth and Cloetingh, 1996). Due to the uplift of the Buda Hills (Kele et al., 2011; Ruszkiczay-Rüdiger et al., 2005b; Wein, 1977) – as part of the TR –, the erosion of Palaeogene rocks was initiated from Pliocene times. Simultaneously, due to the NW-SE trending normal faulting between the uplifting and subsiding
blocks (Fodor et al., 1999), sedimentation continued in the subsiding basinal sectors. It is remarkable that the average sedimentation rate of the Pannonian Basin increased by two and a half times (to 0.78 mm yr\(^{-1}\)) during the Late Miocene compared to the rate during the Early Miocene (0.33 mm yr\(^{-1}\)) (Hámor, 1984; Horváth et al., 1988).

Based on fission track analyses of buried and exhumed rocks along the margins of the Pannonian Basin (Dunkl and Frisch, 2002), it can be assumed that the Buda Hills area was originally covered by several hundreds of meters of Late Miocene sediments. Entrapment temperatures and pressures of fluid inclusions in calcite veins reflects that approximately 800 m of sediments have been eroded since the late Early Miocene (~17 Myr) (Poros et al., 2012).

The onset of inversion gradually migrated towards more internal parts of the system (Fodor et al., 2005a; Tari, 1993). The structural inversion of the Gödöllő Hills was manifested in the folding of the uppermost pre-Quaternary strata (Fodor et al., 2005b) and has been ongoing for the past 4 million years (Ruszkiczay-Rüdiger et al., 2006; Ruszkiczay-Rüdiger et al., 2007). Due to this landscape evolution the recent surface watershed has also been evolving (Ruszkiczay-Rüdiger et al., 2007).

By the Pliocene (~5 Myr) the entire basin had infilled, forming a terrestrial environment (Jámbor, 1989; Juhász, 1994; Magyar et al., 1999; Magyar et al., 2013). The “modern” Danube found its place between the uplifting Transdanubian Range and North Hungarian Range in Pliocene – Pleistocene times (Bulla, 1941; Gábris, 1994; Pécsi, 1959; Ruszkiczay-Rüdiger et al., 2005a; Ruszkiczay-Rüdiger et al., 2005b). In recent times, the river represents the lowest surface elevation (as well as displaying the lowest water table elevation) within the region between the unconfined and confined parts of the system (Mádl-Szőnyi and Tóth, 2015). The incision rate of the river also provides a reasonably good approximation of the degree of uplift, which was calculated to be between 0.02 and 0.06 mm yr\(^{-1}\) for the time interval between 2.4 Myr and 360 kyr, while between 0.23 and 0.14 mm yr\(^{-1}\) in the last 360 kyr of the Pleistocene (Ruszkiczay-Rüdiger et al., 2005b). Thus the river has made an incision of approx. 90 to 200 m (equivalent to the uplift rate of the mountain range) over the last 2.4 Myr.

Travertines, which formed during the Late Miocene (Müller and Magyar, 2008), could be the first indicators of groundwater discharge (Pentecost, 2005). In Pleistocene times (from ~2.5 Myr), travertines formed at the margins of the uplifting hills (Kele, 2009; Scheuer and Schweitzer, 1980). They reflect hydrogeological changes associated with the uplift (Poros et al., 2012), since the younger travertines occur at lower topographic position compared with the older ones (Kele, 2009; Scheuer and Schweitzer, 1988). Moreover, the paleoclimatological and sedimentological studies of Kele et al. (2011) highlighted that travertines of the Buda Hills precipitated from
warmer water (with temperatures between 20 and 65 °C) compared to recent deposits which originated from lukewarm springs (with temperatures between 20 and 28 °C).

**Recent geological and hydrogeological environments**

The connection between the tectonically divided unconfined and confined parts of the BTK is provided by a Mesozoic carbonate suite, which is downfaulted and continues deep on the basin side (below the Pest Plain, see Figure 3b) to the east of the Danube, under a thick Neogene siliciclastic sedimentary cover (Figure 5). The geological structure is strongly controlled by tectonic elements, mainly normal and reverse faults trending in the NW-SE, NE-SW and N-S directions (Fodor et al., 1994).

Triassic (Ladinian to Norian) platform carbonates (dolomites and limestones) constitute the main aquifer of the area with a thickness of 1500–1800 m (Haas, 1988; Wein, 1977). Jurassic and Cretaceous sediments are missing in the BTK area, which were supposedly removed by subsequent erosion from Late Cretaceous to Late Eocene (Wein, 1977). The eroded surface of the Triassic sediments is covered by a Palaeogene transgression sequence (Báldi and Báldi-Beke, 1985) starting with bauxitic clays, followed by Upper Eocene to Lower Oligocene limestone and marls (Kleb et al., 1993). The Early Oligocene is represented by several hundreds of meters of thick anoxic clay (Báldi and Báldi-Beke, 1985; Báldi et al., 1984) and coarse-grained coastal siliciclastic formations. Fine-grained sand and silt deposition took place during the Late Oligocene. Erosion from Miocene times removed parts of the Palaeogene rocks (Wein, 1977). Travertines formed at the margin of the uplifted blocks (Kele et al., 2011; Scheuer and Schweitzer, 1988). In Pleistocene to Holocene times, eolic and fluviatile sediments as well as talus were deposited in addition to travertines (Wein, 1977). The Danube has been depositing its gravel sediments since the Pliocene (Pécsi, 1959; Pécsi, 1991). East of the Danube, the top of the Triassic carbonates is found at a depth of 1500-2000 m or deeper below the surface of Pest Plain (Rónai, 1986), covered by Paleogene to Neogene sediments of variable thickness.

A simplified hydrostratigraphic structure of the BTK was provided by Mádl-Szőnyi and Tóth (2015) based on the geological profile of Fodor (2011) and hydrostratigraphic study of Martinecz et al. (2014) (Figure 5). West of the Danube, the carbonate rocks, characterised by relatively high hydraulic conductivity \(K_h=10^{-4} \text{ m s}^{-1}, K_z=10^{-5} \text{ m s}^{-1}\), are situated close to the surface, sporadically overlain by Tertiary cover formations with a relatively small thickness (up to a 150-200 m) compared to the 3-4 km thick carbonate rocks (Figure 5) facilitating recharge into the carbonates. Therefore, on the regional scale, these deposits can be treated as an unconfined subsystem. East of the Danube, the thick siliciclastic cover can be characterised by very low hydraulic conductivity
(Kx=10^-7 ms^-1, Kz=10^-8 ms^-1; Figure 5), which therefore functions as a confined subsystem (Mádl-Szőnyi and Tóth, 2015).

Flow system boundary conditions

Being located at the north-eastern discharge zone of the Transdanubian Range, the BTK received continuous subsurface inflow from the W-NW by regional and intermediate groundwater flow systems across the carbonate range, which was numerically simulated by Mádl-Szőnyi and Tóth (2015). Evidence of large-scale regional and intermediate flow systems was also provided by the intense artificial intervention of mine dewatering, which has decreased the regional hydraulic heads throughout the reservoir of the Transdanubian Range (Csepregi, 2007; Hőriszt, 1971; Lorberer, 1986), extending as far as the BTK.

The eastern boundary of the system is relatively well defined based on recent studies of Mádl-Szőnyi et al. (2015) and Mádl-Szőnyi et al. (2018). East of the Danube, the Gödöllő Hills area is divided into western and eastern parts by the Szada normal fault (Figure 5) with an approx. 500-1000 m vertical dislocation (Fodor et al., 2005a; Fodor et al., 2005b; Haas et al., 2010; Kiss et al., 1999; Rónai, 1986). This structural element acts as a barrier, since groundwater flow impinges against the low permeability Paleogene-to-Miocene sedimentary sequence of the downfaulted eastern block (Mádl-Szőnyi et al., 2018). Uplift of the Gödöllő Hills within the last 4 million years (Ruszkiczay-Rüdiger et al., 2006) contributed to the change of subsurface pressure conditions (based on Terzaghi, 1925). Moreover, below the Gödöllő Hills, the low-permeability confining formations overlying the carbonate led to restricted recharge on geological time scales and to the development of underpressure conditions in the Oligocene and Triassic-Eocene carbonate formations (Mádl-Szőnyi et al., 2015). These underpressured carbonates further to the east of the Szada fault developed a hydraulic ridge for groundwater flow, and are therefore considered as the eastern hydraulic boundary of the BTK (Mádl-Szőnyi et al., 2018).

Fluids in the system, their natural discharge and cave development

The natural discharge of the BTK is manifested mainly in the form of springs along and in the riverbed of the Danube forming three distinct well-known discharge areas, influenced by tectonic patterns (Alföldi et al., 1968; Erhardt et al., 2017; Erőss et al., 2012a; Erőss et al., 2012b). The discharge along the river was identified in the upper 50 m by a detailed hydraulic evaluation of Erhardt et al. (2017). However, below this depth, the hydraulic potential distribution shows groundwater flow from west to east, which reflects through-flow below the Danube.
Figure 5 – a) Geological cross-section after Fodor (2011 in Mindszenty 2013) b) Simplified hydrostratigraphic structure of the Buda Thermal Karst. Hydrostratigraphic categories based on Martinecz et al. (2014). Hydrostratigraphic values based on Mádl-Szőnyi and Tóth (2015). For trace of the geological cross-section, see Figure 3.
The possible contribution of basinal fluids to the BTK was first proposed by Alföldi (1981) and later supported by the analyses of discharging fluids by Erőss (2010; 2012a) as well as on the mineralogical and fluid inclusion study of Poros et al. (2012). However, the mechanism of basinal contributions to the BTK system in the form of downward leakage from the confining formations to the carbonates was revealed by Mádl-Szőnyi and Tóth, (2015) and Mádl-Szőnyi et al. (2015). Interactions between the carbonate rocks and the fluids, which originated from meteoric infiltration and different basinal sources, contributed to the development and currently active formation of an extensive cave system (Erőss et al., 2012a; Leél-Őssy and Surányi, 2003; Mádl-Szőnyi et al., 2017; Takács-Bolner, 1989), which is characterized by typical hypogenic morphological features and minerals (Leél-Őssy, 1995; Leél-Őssy, 2017).

2.2 Preliminary considerations

2.2.1 Model dimensionality

Real geological systems are complex and groundwater flow processes act in three dimensions. Nevertheless, simplification of geology and subsurface processes necessarily underlies all hydrogeological modelling (Király, 2003; Wainwright and Mulligan, 2005). Representing a 3D system as a two-dimensional cross-section clearly omits some system dynamics. However, depending on the scale of the investigation, the questions to be answered and system characteristics, a two-dimensional approach in some cases could be a suitable choice.

The appropriate dimensionality for simulating groundwater flow can be selected based on the ratio of recharge (R) to hydraulic conductivity (K) of the uppermost subsurface layer because this ratio directly determines the water table configuration (Gleeson and Manning, 2008; Haitjema and Mitchell-Bruker, 2005; Jamieson and Freeze, 1982). For low-relief settings (i.e. with a flank slope < 10°), where the R/K ratio is < 0.15, 2D cross-sectional models may be justifiable since transverse flow (perpendicular to the primary regional topographic gradient) would be generally less than 10% of the total flow. On the other hand, if R/K > 0.15, a 3D approach would be needed.

Based on evaluations in both margins (unconfined, confined) of the studied BTK system, the R/K ratio is below the critical value (Table 1). Moreover, the focus of this study has been directed toward understanding dynamically changing flow regimes and consequent temperature distribution. Therefore, looking for general trends and characteristics of the transient flow system and temperature field, a 2D model is considered a reasonable approach for providing the needed insight.
### 2.2.2 Water table configuration

The current numerical investigation focuses on regional-scale fluid flow and heat transport within the saturated zone of a carbonate system, for which the water table forms the upper surface. Under conditions of differential basin uplift, the water table gradients act as the principal driving forces for groundwater flow (Tóth, 2009). The relation of the water table to surface topography thus becomes a critical factor in shaping the flow system.

In this context, Haitjema and Mitchell-Brucker (2005) offered a simple dimensionless decision criterion to distinguish between recharge- and topography-controlled water table configurations for numerical simulations. Based on the average annual recharge rate ($R$ [md⁻¹]), the average distance between lateral hydraulic boundaries ($L$ [m]), an aquifer shape factor ($m$ [0]; for one-dimensional flow between two parallel surface water boundaries $m=8$, while for radial flow in an aquifer of diameter $L$, $m=16$), and based on the average horizontal hydraulic conductivity ($K$ [md⁻¹]), the average aquifer thickness ($H$ [m]), and the maximum distance between the average surface water levels and the terrain elevation ($d$ [m]) (Figure 6a), the following ratio was defined:

$$\alpha = \frac{R L^2}{m K H d} \quad \text{(Equation 1)}$$

If $\alpha > 1$, the water table is topography-controlled, and should follow a subdued replica of the terrain surface (Haitjema and Mitchell-Brucker, 2005). In this case, groundwater flow is dominated by local circulation in a hierarchically-nested flow domain (Figure 6b). In comparison, for $\alpha < 1$, the water table is recharge-controlled and shows moderate to small degrees of groundwater mounding in response to average recharge. Areas in such settings have subordinate local components of groundwater flow, while the major flow component is regional (Figure 6c) (Haitjema and Mitchell-Brucker, 2005). Recharge-controlled water tables are common in arid, rugged, or high-permeability terrain where actual recharge rates are less than the potential infiltration capacity, and a larger proportion of flow is regional.

<table>
<thead>
<tr>
<th>Annual precipitation (P)</th>
<th>700 mm yr⁻¹</th>
</tr>
</thead>
<tbody>
<tr>
<td>Annual evapotranspiration (E)*</td>
<td>465 mm yr⁻¹</td>
</tr>
<tr>
<td>Recharge ($R=P-E$)</td>
<td>$7.4 \times 10^{-9}$ ms⁻¹</td>
</tr>
<tr>
<td>Hydraulic conductivity (K)</td>
<td>$10^{-4}$ ms⁻¹</td>
</tr>
<tr>
<td>$R/K$ ratio</td>
<td>0.0001</td>
</tr>
</tbody>
</table>

* Evapotranspiration was calculated based on the Turc formula (Turc, 1961)
Due to the higher hydraulic conductivity of carbonate ranges compared to siliciclastic environments at the basin scale, we can expect dominantly recharge-controlled systems in semi- or unconfined carbonate regions (Mádl-Szőnyi and Tóth, 2015). Based on site-specific values of the analogue pilot area, the ratio was indeed $\alpha < 1$, therefore the configuration of the water table was defined as recharge-controlled.

### 2.2.3 Driving forces on groundwater flow

Although a varying water table gradient acts as the principal driving force of gravity-driven regional groundwater flow, effects of other flow generating mechanisms, such as buoyancy, sediment compaction or tectonic compression etc., could be superimposed on the effect of gravity (Garven, 1995; Ingebritsen et al., 2006).
Buoyant convection (or free convection) can occur in geological systems in which the permeability and geothermal gradient are sufficiently high and where a temperature or concentration gradient is strong. In the case of non-isothermal conditions, for example, the relative strength of thermal conduction vs. convection can be estimated by the Rayleigh number \( R_a \), which is a dimensionless ratio that determines the onset of thermal free convection, defined as follows:

\[
R_a = \frac{\alpha_T g \rho^2 c_w k (y^2) \gamma}{\mu \lambda}
\]

where \( \alpha_T \) is the coefficient of thermal expansion for water \( (2.14 \times 10^{-4} °C^{-1}) \), \( g \) is the acceleration due to gravity \( (9.81 \, \text{ms}^{-2}) \), \( \rho \) is the water density \( (1000 \, \text{kgm}^{-3}) \), \( c_w \) is the water specific heat capacity \( (4174 \, \text{Jkg}^{-1}°C^{-1}) \), \( k \) \( (\text{m}^2) \) is the permeability, \( y \) \( (\text{m}) \) is the height of the medium, \( \gamma \) \( (°C\text{m}^{-1}) \) is the vertical thermal gradient, \( \mu \) \( (\text{kgm}^{-1}\text{s}^{-1}) \) is the water dynamic viscosity and \( \lambda \) \( (\text{Wm}^{-1}°C^{-1}) \) is the thermal conductivity of the saturated porous medium.

A Rayleigh-analysis assumes i) convection within a horizontal porous medium situated between two impermeable boundaries perpendicular to the gravity vector, ii) constant salinity and iii) an incompressible fluid. Although in many geological situations these assumptions are violated (Criss and Hofmeister, 1991), the calculation can help to decide whether or not buoyancy effects will arise in a specific case.

Assuming \( \mu=0.0004 \, \text{kgm}^{-1}\text{s}^{-1} \), with \( \lambda=2.5 \, \text{Wm}^{-1}°C^{-1} \), a 4000 m deep carbonate system with \( \gamma=0.05 \, °C\text{m}^{-1} \), then theoretically, a minimum permeability of \( k=5.7 \times 10^{-15} \, \text{m}^2 \) (equivalent to \( K=5.7 \times 10^{-8} \, \text{ms}^{-1} \) assuming a temperature of 10 °C) is required for the onset of buoyancy, based on the critical value \( R_a^* = 4\pi^2 \approx 40 \) (Turcotte and Schubert, 1982).

Comparing this conductivity with the range of hydraulic conductivities of karst limestone, limestone and dolomite \( (2\times10^{-2} - 10^{-6} \, \text{ms}^{-1}) \), with a minimum value of \( 10^{-9} \, \text{ms}^{-1} \) (Domenico and Schwartz, 1990), we can surmise that conditions would indeed be favourable for development of thermal convection cells in the studied 4000 m thick carbonate unit.

Therefore, the influence of a buoyancy-driven force was taken into account in addition to the effect of the GDRGF during all simulations. In case of the pilot area, the groundwater TDS remains below 40 gl$^{-1}$ (Czauner and Mádl-Szőnyi, 2013) and should thus not play a role. While temperature-dependent fluid density and viscosity was included in the model, for simplicity, the effect of density-driven flow due to high total dissolved solids (TDS) concentrations was neglected.
### 2.3 Simulation approach

Simplified, semi-synthetic snapshot models were simulated in a 2D vertical plane using the Heatflow-Smoker finite element model (Molson and Frind, 2017) which couples density-dependent groundwater flow and heat transport. The thermal transport model is based on the solutions to the saturated density-dependent groundwater flow equation, and on a modified form of the advection-dispersion equation.

The continuity equation for flow can be expressed as (Bear, 1972):

\[
\frac{\partial}{\partial x_i} \left[ K_{ij}(T) \left( \frac{\partial \psi}{\partial x_j} + \rho_r(T) \cdot \bar{n}_j \right) \right] = S_s \frac{\partial \psi}{\partial t}
\]  

(Equation 3)

where \( x_i \) are the 3D spatial coordinates (m), \( K_{ij}(T) \) is the temperature-dependent hydraulic conductivity tensor (m s\(^{-1}\)), \( \psi \) is the equivalent freshwater head (m), \( \rho_r(T) \) is the temperature-dependent relative density of water (-), \( S_s \) is the specific storage (m\(^{-1}\)), and \( t \) is time (s). The temperature-dependent fluid density and viscosity functions used to define the hydraulic conductivity term were based on polynomials regressed from data in Weast (1980) over the temperature range 0-100 °C (Molson and Frind, 2017).

The governing thermal transport equation for a porous medium can then be expressed as:

\[
\frac{\partial}{\partial x_i} \left[ (\kappa + \frac{D_{ij}}{R_T}) \frac{\partial T}{\partial x_j} \right] - \frac{\partial}{\partial x_i} \left( \frac{v_i}{R_T} \right) = \frac{\partial T}{\partial t}
\]  

(Equation 4)

where \( T \) is the temperature (°C), \( D_{ij} \) is the hydrodynamic dispersion tensor (m\(^2\)s\(^{-1}\)) as given by Molson et al. (1992), \( v_i \) is the average linear groundwater velocity (ms\(^{-1}\)), \( \kappa \) is the thermal diffusivity (m\(^2\)s\(^{-1}\)) and \( R_T \) is the thermal retardation (-). The thermal diffusivity is defined by

\[
\kappa = \frac{\lambda}{C_0}
\]  

(Equation 5)

where \( \lambda \) is the thermal conductivity of the porous medium (Jm\(^{-1}\)s\(^{-1}\)°C\(^{-1}\)) and \( C_0 \) is the heat capacity (Jm\(^{-1}\)°C\(^{-1}\)) given by:

\[
C_0 = \eta c_w \rho_w + (1 - \eta) c_s \rho_s
\]  

(Equation 6)

where \( \eta \) is the porosity, \( c_w \) and \( c_s \) are the specific heat capacities (Jkg\(^{-1}\)°C\(^{-1}\)) of the fluid (water) and solids, respectively, and \( \rho_w \) and \( \rho_s \) are respective phase densities (kgm\(^{-3}\)).

The bulk thermal conductivity of the porous medium (Jm\(^{-1}\)s\(^{-1}\)°C\(^{-1}\)) can be defined as:

\[
\lambda_0 = \eta S_w \lambda_w + (1 - \eta) \lambda_s
\]  

(Equation 7)

where \( S_w \) being the water saturation, \( \lambda_w \) and \( \lambda_s \) are the phase thermal conductivities (Jm\(^{-1}\)s\(^{-1}\)°C\(^{-1}\)) of the fluid (water) and solids, respectively (Molson and Frind, 2017).
The thermal retardation factor $R_T$ in Equation 4 can be defined as:

$$R_T = \frac{C_0}{\eta \epsilon w \rho w}$$  
(Equation 8)

The model uses deformable rectangular prism elements and the final matrix equations for both the flow and thermal transport problems are solved using an efficient preconditioned conjugate gradient (PCG) solver for symmetric matrices (Schmid and Braess, 1988).

Numerical errors are controlled by observing the grid Peclet and Courant criteria (Daus et al., 1985) given by

$$P = \frac{v \Delta x}{R \kappa + D} \leq 2$$  
(Equation 9)

$$C = \frac{v \Delta t}{R \Delta x} \leq \frac{P}{2}$$  
(Equation 10)

where $\Delta x$ and $\Delta t$ are the grid spacing and time step, respectively.
3 NUMERICAL INVESTIGATIONS

3.1 Conceptual models of geological evolution

The numerical investigations of groundwater flow over geological time scales were placed into realistic geological evolutionary contexts through an example of the BTK. Based on its system evolution, four main phases were distinguished and scenario modelling was carried out in order to examine the effects of tectonic uplift and erosion of confining siliciclastic strata above the carbonates.

The main goal was to gain insight into the effect of decreasing thickness of the low-permeability confining layer on the flow field and heat distribution. A simplified geological and hydrostratigraphic conceptual model was therefore applied. Moreover, with such relatively simple settings, the groundwater flow distribution and heat transport processes are easily comparable for the different evolutionary stages. The basic geometry of the flow domain followed the existing steady-state model domain of Mádl-Szönyi and Tóth (2015). Consequently, simulated changes in the flow field that could lead to changes in heat distribution, as well as identifying the relative importance of gravity and buoyancy could be more easily determined. Therefore, the following conceptual models were developed.

1. As an initial condition for the geological evolution, a fully confined carbonate system was numerically interpreted, characteristic of the Early Late Miocene (approx. 10 Ma) in the pilot area (Stage 1, Figure 7a). An 800 m thick low-permeability sedimentary cover was assumed to overlie the 3200 m thick permeable carbonate unit, which was approximated based on entrapment temperatures and pressures of fluid inclusions in calcite veins measured by Poros et al. (2012) for the pilot area. A flat water table coinciding with the ground surface was assumed to represent the initial condition before the area became subaerially exposed due to regression of Lake Pannon (Figure 4).

2. In the next evolutionary stage (Stage 2, Figure 7b), vertical uplift of the western block began and in parallel, recharge of the system began by meteoric water infiltration. This phase represents Early Pliocene (5.3 – 3.6 Ma) conditions in the context of the BTK. Due to this evolutionary step, the thickness of the cover formation along the western subsystem was halved by erosion. In parallel, sediment accumulation continued in the eastern subbasin due to re-deposition of the eroded formations from the neighbouring elevated areas. Due to the slightly elevated water table beyond the uplifting western part,
open lateral boundaries can be assumed which allowed water inflow from the western boundary and in parallel, water outflow along the eastern boundary.

(3) Stage 3 denotes these changes, which occurred during the Late Pliocene (3.6 – 2.58 Ma) at the BTK (Figure 7c). Uplift of the eastern subsystem was initiated from approx. 4 Ma, which lead to the differentiated increase of topographic elevations and development of system boundaries. Assuming that sediment accumulation has kept pace with sediment compaction along the eastern part of the system, the thickness of the cover formation was assumed to remain 1500 m during Stage 3 and 4. Additionally, an erosion base evolved between the uplifting blocks (coinciding with what would eventually become the Danube basin in the case of the pilot area), which also represents the minimum water table elevation within the system. Due to topographic changes caused by further uplift of the western block and recently initiated uplift of the eastern block, head differences increased along the water table.

(4) Additional uplift along the western sub-basin lead to the complete erosion of the cover unit above this area, which produced unconfined conditions, represented by the last evolutionary stage (Stage 4, Figure 7d). This stage reflects the most recent site characteristics, including conditions observed today in the pilot area. The eastern sub-basin remains confined, since uplift and erosion of thicker sedimentary cover began later.

For simplicity, and bearing in mind the main goal of the numerical investigation being process understanding, the thickness of the siliciclastic cover above the eastern carbonate subsystem was assumed to be constant during the simulated stages.
Figure 7 – Conceptual models of the numerically investigated geological evolutionary stages. a) Stage 1: Fully confined carbonate phase, b) Stage 2: Uplift and erosion of the west subregion and sedimentation along the east subregion, c) Stage 3: Development of system boundaries, d) Stage 4: Completely unconfined condition over the west subregion. (ψ: equivalent freshwater head)
3.2 Input parameters, initial and boundary conditions of the models

Following the EPM approach, fracture networks and karstic channels were not integrated into the model as discrete elements, since the scale of fracture apertures (on the order of µm to cm) is not comparable with the regional scale of the model domain (on the order of several tens of km length). However, large-scale and systematic variations in aquifer properties cannot be ignored, since they are heterogeneous, anisotropic and transient.

Based on globally compiled data, Ehrenberg and Nadeau (2005) revealed that both carbonate and siliciclastic formations generally show an apparently linear decrease in porosity with increasing depth due to the main burial-diagenetic processes, which led to a gradual porosity occlusion. Moreover, carbonate reservoirs have a greater relative proportion of high hydraulic conductivity at low porosities, which may reflect greater incidence of fracture permeability in the carbonate reservoirs, instead of fabrics composing the rock matrix.

The role of regional-scale systematic heterogeneity of K on basin groundwater flow has been discussed by Jiang et al. (2009). Based on their results, the development of local versus regional flow systems is sensitive to the rate of decay in K with depth, since a nonlinear depth-dependent decrease in K enhances penetration depths of local flow systems by decreasing the intensity of the deeper flow systems. Therefore, the depth-decay of K should not be neglected when numerically analysing hydrogeologic systems related to regional groundwater flow.

Taking into consideration the scale-dependency of porosity and hydraulic conductivity values revealed by Király (1975), the observed hydraulic properties of the carbonate unit were slightly increased in the model to account for regional fracture networks and interconnected karstic channels which tend to increase the hydraulic conductivity and porosity on the regional (aquifer) scale compared to the local (borehole) scale.

All of these considerations were taken into account for defining input parameters of the model scenarios. For reasons of comparability of processes in the different evolutionary stages, hydraulic conductivity and porosity values of the semi-synthetic models were constant for all tested stages i.e. their transient nature was neglected. The parameters were estimated based on global physical properties of the carbonate and siliciclastic reservoirs (Ehrenberg and Nadeau, 2005). Additionally, information from site-specific hydrostratigraphic and numerical studies of the pilot area ( Mádl-Szőnyi and Tóth, 2015; Martinecz et al., 2014) were also considered.

In order to take into account the unique features of karst systems, an exponential decrease of hydraulic conductivity was defined for the carbonate suite, with the horizontal conductivity (K_x) ranging from $10^{-4}$ m s$^{-1}$ at the top to $10^{-6}$ m s$^{-1}$ at the bottom of the section. This change of hydraulic conductivity integrates both the decrease of K with depth, and alteration of the shallow conductive
zone by near-surface karstification processes. Since the main focus of the simulation was on the flow and heat transport processes acting in the carbonate unit, and since the hydraulic conductivity contrast between the carbonate and the overlying cover unit is high (3 orders of magnitude), the decrease of K with depth in the siliciclastic cover unit was neglected, and a uniform horizontal hydraulic conductivity (Kx) of $10^{-7}$ m s$^{-1}$ was defined for the cover. Anisotropy of the units was characterized by a one order of magnitude lower vertical conductivity (Kz) (thus assuming an anisotropy ratio Kz/Kx = 0.1) (Table 2).

A uniform bulk (saturated) thermal conductivity of 1.4 W m$^{-1}$°C$^{-1}$ for the siliciclastic cover and 2.1 W m$^{-1}$°C$^{-1}$ for the carbonate unit were assumed, derived from site-specific data of Rman and Tóth (2011) and Mádl-Szőnyi and Tóth (2015). Basic physical properties of the formations such as density and specific heat capacity were defined based on Waples and Waples (2004) and are summarized in Table 2.

Boundary conditions for groundwater flow vary depending on the different geological stages, as described below.

(1) In Stage 1 (Figure 7a), the lower boundary was defined based on the hydrostratigraphic section of the analogue area (Figure 5), where low permeability Palaeozoic formations underlie the carbonate unit, and therefore the bottom of the system can be treated as a no-flow boundary due to the high (4 orders of magnitude) hydraulic conductivity contrast (Martinecz et al., 2014). This lower boundary condition was assumed to be constant during the evolution of the system. For the theoretical scenario of this initial system state, geological and hydrogeological information was not available regarding the probable margins of the system. Therefore, the lateral boundaries of the section were simply defined as being closed by assuming no-flow boundaries as a base case in order to delineate a subsurface area with a homogeneous cover of siliciclastic sediments. At the top, a uniform and flat water table was assumed with a hydraulic head ($\psi$) of 0 m, which represents the conditions before the area became subaerially exposed.

(2) In Stage 2 (Figure 7b), the eastern part of the system is characterised by a uniform flat water table as in the previous stage of the evolution. However, a higher water table ($\psi$=10 m) would be expected beyond the uplifting western part of the simulated domain, derived from current water table elevations along this boundary, assuming gradual uplift. These conditions would induce a hydraulic gradient between the western and the eastern part of the system. Based on this consideration, along the western lateral boundary, a water influx was assigned and in parallel, water outflow was assumed along the eastern lateral boundary (Table 2).
In Stage 3 (Figure 7c) the upper flow boundary was a fixed-head boundary with a linear decrease of the water table from the left boundary (where $\psi=20$ m) to the minimum elevation point (where $\psi=0$ m) at the river, as well as a linear increase of the water table to the right boundary (where $\psi=15$ m). Due to the higher water table differences along the western boundary, which induces a higher hydraulic gradient, lateral influx increased compared to the previous stage. Considering the geological evolution of the pilot area, the eastern lateral boundary was assumed to be a no-flow boundary due to the development of a hydraulically closed watershed east of the system.

In Stage 4, the maximum height of the water table is assumed to be 31 m at the left boundary and 26 m at the right boundary, relative to the minimum elevation point (where $\psi=0$ m) based on the recent water table configuration of the pilot area. Increased water influx was assumed along the western boundary, while the eastern lateral boundary was handled as a no-flow boundary as in the previous stage of geologic evolution.

A constant ground surface temperature of 10 °C was assumed in all cases based on an estimated mean annual temperature representative of the pilot area over the geological time frame. For simplicity, effects of variable surface temperature due to climatic change were neglected. Across the bottom boundary, a heat flux of 100 mWm$^{-2}$, characteristic recent time for the analogue pilot area, was defined based on Lenkey et al. (2002). An initial basal temperature of 100 °C was used, calculated from an average geothermal gradient of 40 °Ckm$^{-1}$, taking into account the cooling effects of infiltrating meteoric water. Lateral boundaries were set as zero temperature-gradient boundaries, thus assuming no conductive heat transfer in the cases with no-flow lateral boundaries, and assuming advective heat flow is dominant across open flow boundaries (Table 2).

The 25 km wide and 4 km deep model domain was subdivided into a regular network of 100 m×100 m rectangular prism finite elements (using 250×40 elements, and 1 element wide in the transverse dimension). The simulations were run over 220 kyr, with a time step of 10 yr. Hydraulic head distributions and the corresponding temperature fields of all scenarios were plotted at 220 kyr. The simulated time interval was verified sufficient to reach a quasi-steady state solution – with temporally repeating similar patterns over geologic time scales – for each stage.
### Table 2 – Summary of input parameters, initial and boundary conditions for the simulation scenarios

<table>
<thead>
<tr>
<th></th>
<th>Stage 1</th>
<th>Stage 2</th>
<th>Stage 3</th>
<th>Stage 4</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Boundary conditions for groundwater flow</strong></td>
<td></td>
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<td></td>
</tr>
<tr>
<td>Left</td>
<td>q=0 ms⁻¹</td>
<td>q=10⁻¹⁰ ms⁻¹</td>
<td>q=2×10⁻¹⁰ ms⁻¹</td>
<td>q=3×10⁻¹⁰ ms⁻¹</td>
</tr>
<tr>
<td>Right</td>
<td>q=0 ms⁻¹</td>
<td>q=(-10⁻¹⁰) ms⁻¹</td>
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<td></td>
</tr>
<tr>
<td>Bottom</td>
<td>q=0 ms⁻¹</td>
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<td></td>
</tr>
<tr>
<td>Top</td>
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<td>ψ(at 0 km)=20 m</td>
<td>ψ(at 0 km)=31 m</td>
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<td><strong>Boundary conditions for heat transport</strong></td>
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<tr>
<td>Bottom</td>
<td></td>
<td>T=10 °C fixed temperature</td>
<td></td>
<td>T=10 °C fixed temperature, zero temperature gradient at the minimum elevation point</td>
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<tr>
<td>Top</td>
<td>T=200 °C</td>
<td>temperature solution of Stage 1</td>
<td>temperature solution of Stage 2</td>
<td>temperature solution of Stage 3</td>
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*Water density is temperature-dependent*
3.3 Evolution of fluid flow patterns and heat distribution over geological time scales

3.3.1 Stage 1 – A fully confined initial system stage

As the initial condition for the geological evolution in Stage 1, a fully confined carbonate system was assigned in the model, overlain by low conductivity siliciclastic sediments (Figure 7a). A flat water table coinciding with the ground surface was assumed representative of the initial condition before the area became subaerially exposed.

Flow pattern

Since the water table is flat (representing lake level) in this stage, there are no imposed hydraulic gradients which could generate topography-driven flow (Figure 8a). Nevertheless, complex buoyancy-driven hydrothermal convective flow systems evolve within the permeable carbonate unit (Figure 8b), which are maintained due to the heat-insulating role of the low-conductivity siliciclastic confining formation (as seen in the temperature field of Figure 8c). Convective flow cells are easily formed as the average Rayleigh number \( R_a = 350 \) exceeds the critical value by at least a factor of 10. Since the Rayleigh number is very high, the convection cells are unstable in the sense they do not settle down to a steady-state configuration. Therefore, some cells gradually dissipate with time while new ones are born, eventually reaching a quasi-steady state pattern with temporally repeating similar patterns within the 220 kyr time frame. This setting leads to the development of a vigorous, dynamic system with transient convection cells, which divide the flow field into three separate flow systems \( S_1, S_2, S_3 \), see Figure 8a) after 220 kyr. Although the overlying sediments are much less permeable than the carbonates, some inflow and outflow still occurs across the flat water table due to the underlying thermal gradients (Figure 8a). These recharge or discharge fluxes, however, would be relatively low. The maximum groundwater flow velocity is \( 1.9 \times 10^{-7} \text{ ms}^{-1} \) within the carbonate unit.

Heat distribution

In this initial stage of geologic evolution, the flow and temperature field is clearly dominated by natural thermal convection, with maximum temperatures at the base reaching 85-90 °C. After 220 kyr, six upwellings have developed, originating from hot spots along the base \( \text{(U1-U6, see Figure 8b), and which have a complex distribution across the system. Cells are born from these hot spots and the water temperature decreases by approx. 40 °C during its upwelling. Temperature differences within the cover layer are relatively low, and heating effects of convection cells within the carbonate are limited to the base of this layer.} \)
Figure 8 – Simulation Stage 1 (no uplift), generated only by thermal buoyancy, showing a) shape of the water table, b) the quasi steady-state hydraulic head distribution (m) and c) the corresponding temperature field, after 220 kyr. The (same) quasi-steady flow system after 220 kyr is superimposed in both cases. Dashed lines represents boundaries between separated convection cells S1, S2 and S3. Monitoring points are identified for further analyses (Chapter 3.3.5) as M-1, M-2, M-3 (at 3000 m depth at 2, 12.5 and 23 km distances, respectively) and M-4 (at the top of the section at 15 km distance). U1, U2, etc. represent the upwellings. Ra identifies the location and value of the maximum Rayleigh number within the carbonate unit.
3.3.2 Stage 2 – Tectonic uplift with erosion and sediment accumulation

Since vertical uplift of the western block began, the thickness of the cover formation along the western subsystem has been reduced by erosion. On the relatively lower, eastern side of the system, sediment accumulated concurrently with uplift of the western block, which increased the thickness of the low permeability confining formations in this area. Due to the slightly elevated water table beyond the uplifting western part, a hydraulic gradient develops between the two domains. Open lateral boundaries were thus assigned in the model which allow water inflow from the western boundary and water outflow along the eastern boundary.

**Flow pattern**

First, if we take into account only the effect of gravity as the driving force, the flow pattern is relatively simple, groundwater flows from the elevated western sub-basin toward the eastern part of the system characterised by a flat water table. Groundwater discharge takes place along the entire eastern sub-system due to its relatively lower topographic position. The flow field consists of three flow systems, namely S1 which recharges across the western cover layer and S2 which is fed by regional groundwater inflow across the western lateral boundary (Figure 9b). A stagnation point has developed at 17.5 km distance (SP, Figure 9d). Hydraulic gradients within the domain are low, since the induced hydraulic head differences (10 m) are very low compared to the length (25 km) and depth (4 km) of the system. Accordingly, groundwater flow velocities have a magnitude of $10^{-10} - 10^{-9}$ m s$^{-1}$.

Since the average Rayleigh number ($R_d$) is between 210 along the eastern block (which has decreased compared to 350, characteristic of Stage 1) and 450 along the western block (which has increased compared to 350, characteristic of Stage 1), thermal convection is still important within the carbonate (depending on the thickness of the confining formation), and thus including coupled gravity and buoyancy flow significantly changes the generated flow pattern. However, the extent of recharge and discharge regions has remained the same, with regional through-flow within the lower parts of the carbonate system restricted by the developed convection cells (Figure 10c), which has therefore eliminated the D2 discharge zone.

In this convection-dominated system, maximum flow velocities increased by 2-3 magnitudes to $4.5 \times 10^{-7}$ m s$^{-1}$ compared to the gravity-dominated case, which reflects the greater importance of buoyancy on flow dynamics compared to the gravity component.

The limited thickness of the siliciclastic cover along the western block compared to the eastern side has allowed more intensive water infiltration into the system. Convection cells have evolved here as well and have shifted slightly towards the eastern part of the system. Nevertheless, the number of upwellings has decreased from 6 to 4 compared to Stage 1.
Heat distribution

Due to the greater thickness of the confining layer above the eastern block and the slightly eastward-shifted cells, the average temperature within the carbonate increased by approx. 15 °C compared to the previous stage (from 50 °C, characteristic of Stage 1 to 65 °C during Stage 2), with elevated maximum temperatures at the base reaching 98-99 °C (compared to the maximum temperature of 85-90 °C in the previous stage). An approximately linear increase of temperature with depth within the thick cover reflects dominantly conductive heat transfer within this unit (Figure 9d).

Figure 9 – Simulation Stage 2 (limited uplift of western block) showing a) shape of the water table, b) the steady-state hydraulic head distribution and flow patterns generated only by the water table topography (purely gravity-driven, no density effect), c) the quasi steady-state hydraulic head, and d) the temperature field, from a single otherwise identical simulation after 220 kyr, but considering both gravity and buoyancy. The (same) quasi-steady flow system after 220 kyr for the coupled cases (c & d) is superimposed on both plots. R shows location of recharge area, while D1 and D2 show locations of discharge areas. Dashed lines represent boundaries between separate flow systems S1 and S2. U1, U2, etc. represent the upwellings. Ra shows the location and value of the maximum Rayleigh number within the carbonate unit. SP represents the location of the stagnation point.
3.3.3 Stage 3 – Development of the system boundaries

Due to topographic changes caused by further uplift of the western block and initiated uplift of the eastern block, head differences increased along the water table.

Flow pattern

Taking into account only the effect of gravity as the driving force, groundwater flows from the elevated marginal areas to the erosion base in accordance with the hydraulic head differences and hydraulic conductivities. Due to the initiated eastern uplift, a new recharge zone (R2) has developed (Figure 10b). The extent of recharge areas is proportional to the hydraulic gradient along the water table. The flow field is divided into three systems, namely S1 which recharges across the western cover layer, S2 which is fed by regional groundwater inflow across the western lateral boundary, and S3 which recharges across the eastern cover layer (Figure 10b). The stagnation point within the eastern cover layer (which developed during Stage 2, Figure 9d) has shifted toward the boundary between the two sub-systems, to 15.5 km (SP, Figure 10). Groundwater flow velocities have a magnitude of $10^{-10} - 10^{-9}$ ms$^{-1}$.

Nevertheless, the coupled density-dependent flow system in Stage 3 still reflects the dominance of buoyancy as the main driving force, with an average Rayleigh number $R_a$ still relatively high (between 210 and 500 within the carbonates). Buoyancy has significantly modified the flow field by restricting regional through-flow within the lower parts of the carbonate, as also occurred during Stage 2. Due to the induced hydraulic head difference between the eastern boundary and the minimum water table elevation at 15 km, the groundwater discharge zone has been reduced to between 9 km and approx. 23.5 km. The flow penetration depth and extent of the S3 flow system has also been significantly reduced compared to the pure gravity-induced case, which can be attributed to the strong buoyancy forces below the cover layer within the carbonate.

The number of upwellings was not affected by further uplift and development of the R2 recharge area along the eastern sub-system. However, the gravity-driven flow component has increasing importance in determining the movement and shift of the convection cells (Figure 10d). Maximum flow velocities have slightly increased to $5.2 \times 10^{-7}$ ms$^{-1}$ compared to the previous stage.

Heat distribution

More intensive water infiltration into the system due to the thinned cover along the western part of the system leads to increased cooling in this area. Average temperatures decreased from approx. 45-50 °C (in Stage 2, Figure 9d) to approx. 25-30 °C within the carbonate in the left part, increasing the temperature contrast between the two sub-systems. The maximum temperature
below the warmer eastern part of the system (where the cover formation is thicker) also decreased from 99 °C (in Stage 2, Figure 9d) to 89 °C (Figure 10d).

Figure 10 - Simulation Stage 3 (uplift of both blocks) showing a) shape of the water table, b) the steady-state hydraulic head distribution and flow patterns generated only by the water table topography (no density effect), c) the quasi steady-state hydraulic head, and d) the temperature field, from a single otherwise identical simulation after 220 kyr, but considering both gravity and buoyancy. The (same) quasi-steady flow system after 220 kyr for the coupled case (c & d) is superimposed on both plots. R1 and R2 show locations of recharge areas, D1 and D2 show locations of discharge areas. Dashed lines represent boundaries between separate flow systems S1, S2 and S3. U1, U2, etc. represent upwellings. Ra shows location and value of the maximum Rayleigh number within the carbonate unit. SP represents the location of the stagnation point.
3.3.4 Stage 4 – Recent state at the margin of unconfined and confined carbonate

In Stage 4, which represents current conditions in the BTK pilot area, further uplifting of the western part has led to complete erosion of the cover layer, which produced unconfined conditions along this sub-system, and led to large-scale changes in flow patterns and the associated heat distribution.

Flow pattern

Increased infiltration from the western side across the unconfined carbonate resulted in an asymmetric flow pattern (Figure 11b). In the case of pure gravity-induced flow, the boundary between groundwater flow systems S1, S2 and S3 converges at 15 km (at the minimum water table elevation). The discharge zone of the regional S2 flow system is significantly reduced (from 2.5 km, characteristic in Stage 3 to less than several hundred meters in Stage 4). Due to the increased water table elevation within the eastern sub-system (26 m compared to the 15 m in Stage 3), groundwater leaks through the thick cover layer and reaches the carbonate unit (Figure 11b).

Although the Rayleigh number is 560 within the uncovered western sub-system, the importance of buoyancy is relatively less important in controlling groundwater flow within this sub-system. The density-dependent flow system decreased the penetration depth of the S1 flow system, increased the extension of the discharge zone of the regional flow system S2 (Figure 11b) and in parallel, restricted groundwater leakage from the cover layer into the carbonate unit.

The uplift causes the main character of the flow pattern to evolve from buoyancy–driven flow to dominantly gravity-driven groundwater flow (Figure 11c). This is particularly evident along the uncovered western part of the system, where flow intensity has increased due to the high permeability of the carbonates and from increased meteoric infiltration. The highest flow rates ($V_{\text{max}} = 9 \times 10^{-7} \text{ m s}^{-1}$) are in the upper part of the permeable carbonates within the unconfined sub-system, where cooling of the system has therefore significantly progressed. However, conditions over the confined eastern part of the system (where $R_a \approx 210$ within the carbonates) are still favourable for the development of convection cells.

Heat distribution

The asymmetric flow pattern is also attributed to the more intense meteoric infiltration over the unconfined part of the system compared to the confined part. As a consequence, average temperatures decreased from 25-30 °C in Stage 3 (Figure 10d) to approx. 12 °C within the upper section of carbonate in the unconfined part (Figure 11d). Although the maximum temperature
below the eastern part of the system decreased from 89 °C (during Stage 3) to 80 °C, there is nevertheless significant heat accumulation compared to the cold eastern sub-system.

Figure 11 – Simulation Stage 4 (additional uplift of western block) showing a) shape of the water table, b) the hydraulic head distribution and flow patterns generated by only the water table topography, and in c) and d) an otherwise identical simulation after 220 kyr, but considering both gravity and buoyancy, showing c) the quasi steady-state hydraulic heads and d) the temperature field. The (same) quasi-steady flow system after 220 kyr for the coupled case (c & d) is superimposed on both plots. R1 and R2 show locations of recharge areas, D1 and D2 show locations of discharge areas. Dashed lines represent boundaries between separate flow systems S1, S2 and S3. U1, U2, etc. represent the upwellings. Ra shows the location and value of the maximum Rayleigh number within the carbonate unit.
3.3.5 Interpretation and discussion

Hydraulic conditions during system evolution

Regional-scale changes in the water table elevation due to system evolution led to modification of the subsurface potential field. As a consequence, the extent of recharge and discharge areas changed, and in parallel, groundwater outflow rates were modified.

Tectonic uplift contributed to the development of a 17.4 km wide discharge zone during Stage 2 due to the evolved hydraulic gradient along the water table. As the topographic gradient increases (see boundary conditions in Table 2), the spatial extent of the groundwater discharge zone gradually decreases with system evolution from 17.4 km (Stage 2) to 15 km (Stage 3) and 13 km (Stage 4). In parallel, the groundwater discharge rate at the margin of the confined and unconfined sub-systems increased significantly by approx. 3 orders of magnitude from $q_z=1.4\times10^{-10}$ ms$^{-1}$ (Stage 2) to $q_z=1.8\times10^{-7}$ ms$^{-1}$ (Stage 4) (Figure 12). The change in the recharge rate also can be followed along the water table.

Dominant driving forces of the evolutionary stages

Topography-driven flow is generally considered to be dominant in uplifted sedimentary basins (Freeze and Witherspoon, 1967), and it is commonly assumed to overwhelm the buoyancy force since the former typically leads to a maximum flow rate of 1–10 m yr$^{-1}$ (approx. $3\times10^{-8}$ ms$^{-1}$ – $3\times10^{-7}$ ms$^{-1}$) (Garven, 1995; Garven and Freeze, 1984a; Garven and Freeze, 1984b), while the latter usually approaches only 1 m yr$^{-1}$ (approx. $3\times10^{-8}$ ms$^{-1}$) (Evans and Nunn, 1989).

Changes in relative importance of gravity and buoyancy during the four evolutionary stages can be followed along three vertical profiles located at distances of 2 km, 15 km and 23 km from the left boundary of the system, which provides useful insight into the coupled gravity-buoyancy-controlled system behaviour (Figure 13). The three profiles represent recharge, discharge and recharge areas, respectively, in the recent system state (Stage 4), and were plotted at 220 kyr, as in the 2D simulated flow patterns and temperature fields (Figure 8, Figure 9, Figure 10, Figure 11). Because the coupled system is thermally unstable, a final steady-state condition is never reached but it eventually settles down to a quasi-equilibrium state in which convection cells develop and disappear with some regularity. These profiles therefore represent snapshots of a transient progression at 220 kyr, and are only suitable for determining relative conditions and processes acting during system evolution. Nevertheless, several interesting trends can be seen.
Figure 12 – Variations of vertical Darcy flux along the water table during the different geological evolutionary stages. Positive vertical Darcy fluxes represent upward flow, reflecting groundwater discharge (D) along the water table. Negative vertical Darcy fluxes indicate downward flow, reflecting groundwater recharge (R). Vertical Darcy flux at 15 km distance indicated by $q_z$. (Note the different scale of $q_z$ on the vertical axis during the different stages.)
Following Equation 3, contour plots of the equivalent freshwater head ($\psi$) cannot be used alone to infer flow directions since the driving force also includes the relative density term. Therefore, to gain insight into the relative importance of gravity and buoyancy as driving forces during the different evolutionary stages, the ratio of the vertical hydraulic gradient (of the equivalent freshwater head) to relative density, (i.e. $\nabla_z(\psi)/\rho_r$; see also Equation 3) was plotted vs. depth (Figure 13). Since the relative density in these cases is always negative, if this ratio is large and negative, then flow is downward (ex. in the recharge zones at 2 km and at 23 km; Figure 13a and Figure 13c, respectively), while large positive ratios imply upward flow (ex. Stage 4 at 15 km representing discharge to the erosion base; Figure 13b). In both cases of high positive or high negative ratios, flow is dominated by gravitational forces (since $|\nabla_z(\psi)| >> |\rho_r|$). Ratios near zero imply that vertical gravity forces are low compared to thermal buoyancy (since $|\nabla_z(\psi)| << |\rho_r|$), although horizontal hydraulic gradients could still be dominant.

In Stage 1 at all profile locations, above about 1000 m elevation, the ratio of vertical hydraulic gradient to the relative density ($\nabla_z(\psi)/\rho_r$) is negative (Figure 13). While this suggests downward gravity-dominated flow, the relatively low hydraulic conductivity of the continuous confining layer in Stage 1 limits any significant flow across this layer (see Figure 8). Below about 1000 m in almost each stage and location, the ratio of vertical hydraulic gradient to the relative density is near zero, representing relatively strong buoyancy which induces the hydrothermal convection cells seen in Figure 8, Figure 9, Figure 10 and Figure 11. However, in Stage 4 at 2 km, gravity-dominated downward flow (i.e. where $\nabla_z(\psi)/\rho_r < 0$) extends significantly deeper, to a depth of about 3000 m due to the high water table elevation within the unconfined left part of the system (Figure 13a).

During Stage 2, 3 and 4 at 15 km, (Figure 13b), the effect of vertically upward gravity-dominated flow is clear, since the ratio ($\nabla_z\psi/\rho_r$) becomes strongly positive where water discharges to the erosion base. Similarly, upward flow during Stage 2 at 23 km indicates groundwater discharge due to the lower water table elevation compared to the western part of the system (Figure 13c, see also Figure 9).

As the results have highlighted, the effect of gravity can be completely attenuated within the carbonate by the presence of an uppermost low-permeability layer, beneath which fluid flow is clearly controlled by thermally-driven free convection, in agreement with the results of the numerical experiments of Yang et al. (2010). On the other hand, within the uncovered sub-system of Stage 4, the evolved slope of the water table is more important than buoyancy in controlling the fluid flow system, and upwelling is forced by the regional hydraulic gradient, analogous to acting in homogeneous unconfined aquifer, as described by Cserepes and Lenkey (2004).
Figure 13 - Total driving force gradient for flow in the vertical direction at 2 km, 15 km and 23 km distances of the different stages (S1, S2, S3 and S4), respectively. Horizontal axes show the ratio of vertical hydraulic gradient ($\nabla \psi$) to relative density ($\rho_r$).

Variations of temperature with depth along the three vertical profiles are shown in Figure 14. At the 2 km profile, a significant decrease in temperature can be seen due to direct recharge of cooler meteoric water as the west part of the system is uplifted and becomes unconfined during Stage 4 (Figure 14a). Below the constantly confined right part of the system at 23 km (Figure 14c), the temperature has risen in Stage 2, 3 and 4, since the confining layer has become thicker here and thus its insulating effect increases over time. However, during Stage 4 the temperature is lower compared to Stage 2 and 3 (Figure 14c) due to the cooling effect of meteoric water infiltration through the unconfined part of the system. In the profile at 15 km, higher temperatures (>30 °C) in the shallow subsurface during Stage 2 and 3 indicate discharge of groundwater heated from the deeper part of the system, while decreased temperatures during Stage 4 reflects discharging cool water arriving from the west part of the system (Figure 14b).
In the shallow subsurface through the confining layer at 2 km (Figure 14a), the temperature increases roughly linearly with depth (0 to -1000 m in Stage 1 and 0 m to -400 m in Stage 2 and Stage 3). At 23 km (Figure 14c), a very similar linear trend is also evident in the upper approx. 1000 m during Stage 1, which extends even deeper through the thicker confining layer in Stage 2, 3 and 4 (0 to -1500 m). A linear thermal gradient is a result of the dominance of conductive heat transfer, since the Rayleigh number ($R_a=5$) in this low-permeability layer remains below the critical value ($R_a^*=40$) and thus convection cells cannot form. In comparison, the corresponding temperature profiles within the deeper carbonate unit are non-linear, reflecting the additional effect of convective heat transfer, since the Rayleigh number in this unit ($R_a >130$) significantly exceeds the critical value. Towards the base of all profiles (below about -3000 m), the temperature increase with depth is again roughly linear, with about the same temperature gradient in all profiles, being controlled by the imposed geothermal flux and thermal conductivity.
Therefore, the change in temperature with depth is in accordance with the geothermal gradient – characteristics for the area – only in the low-permeability cover formation in the shallower part of the section, as well as at the bottom of the carbonate (Figure 14), where the hydraulic conductivity is lower due to its decrease with depth.

At the discharge area of the system, the vertical temperature gradient deviates from the 40 °C km\(^{-1}\) geothermal gradient (Figure 14b), i.e. from the case of pure conduction. In agreement with the results of An et al. (2015), the larger the degree of convection, the more significant is the deviation from the geothermal gradient and from the pure conduction case.

The temperature distribution of the system is dynamically changing, where cyclic temperature variations at the model base (at 3 km depth, Figure 15) are caused by the stage-specific convection cells (Figure 8c, Figure 9d, Figure 10d, Figure 11d), which also affects the temperature variations at the discharge point of the system (located at the top of the section at 15 km, Figure 15). In this study, however, the simulated temperatures at the 15 km monitor point, which is located within the several-hundred-meter-wide discharge area (corresponding to the Danube River in case of the BTK pilot area), may not be representative, since some numerical dispersion is expected due to the high velocities and rapid mixing of waters of significantly different temperatures.

The approx. 35 kyr period in Stage 1 (Figure 15a) decreases to approx. 15 kyr in Stage 4 (Figure 15d), thus suggesting that the period of cyclic temperature variations decreases during system evolution. This decreasing period (or increasing frequency) of temperature oscillation could be attributable to the more efficient meteoric water infiltration through the reduced thickness of the left cover and the increased differences along the water table. These changes lead to an increase of flow velocities (ex. \(V_z(\text{max})\) increases from \(10^{-7}\) ms\(^{-1}\) in Stage 1 to \(8 \times 10^{-7}\) ms\(^{-1}\) in Stage 4) and to the development of a more dynamic flow system. The highest temperature at the monitoring points is reached during Stage 2 due to the combined effect of the onset of gravity forces on groundwater flow and the insulating role of the thick cover formation along the eastern sub-system.

In the recent state of the system (Stage 4), temperature oscillation occur with a period of approx. 15 kyr, and with an amplitude of 25 °C at the bottom of the carbonate (see M-3 monitor point in Figure 15d). On the other hand, the amplitude of temperature oscillations is only approx. 1-2 °C at the discharge point of the system. This indicates that a major part of discharging groundwater likely originates from the unconfined sub-system areas, which led to overwhelming of the transient effects of convection cells.
Figure 15 – Simulated temperature oscillations over the 220 kyr simulation time at three monitor points along the bottom of the system at 2 km (M-1, below the left part of the system which became unconfined), 12.5 km (M-2, in the middle of the section), 23 km (M-3, below the constantly confined part of the system); and along the top of the system at 15 km (M-4, at the discharge point of the system) (see Figure 8). Horizontal bars with times (kyr) represent the mean periods of the respective temperature oscillations.
3.4 Sensitivity study

Since the numerical investigation is based on simplified, semi-synthetic snapshot models which cover long geological time scales, the ability to validate the results is limited in the early evolutionary stages due to the lack of direct data (regarding e.g. the exact topography and groundwater level, physical properties of the geological formations, thermal conditions, etc.). Therefore, the influence of key variables was investigated by a sensitivity study in order to evaluate the relative importance and effects of different input factors on the model output and results.

Stage 1 served as a basis for the sensitivity study since it is a simple horizontal layer, therefore cellular organization of 2D convective flow and its effects on temperature distribution can be easily followed due to the lack of a gravity-driven flow component. A sensitivity analysis is also performed in the case of Stage 4 since it represents the recent (current) state of the system, therefore results can be discussed with site-specific observations and measurements and compared to previous site-specific conceptual models developed by other authors.

For each of the Stage 1 and 4 cases, the sensitivity analysis proceeded by changing one variable at a time from their respective ‘base case’ parameter list summarised in Table 2. Comparisons between the perturbed cases of each of Stage 1 and 4 with their respective equivalent ‘base case’ (Table 2 parameter set) were made with respect to flow patterns, the period of temperature oscillation over the 220 kyr simulation time at the monitor points, and the maximum temperature and flow velocity over the 220 kyr simulation time.

Changes in control output parameters ($T_{\text{max}}$, $V_{x\text{(max)}}$, $V_{z\text{(max)}}$) were considered as having significantly changed, if the variation was higher than ±30%. An overall sensitivity of the system on each selected parameter was evaluated using the following criteria:

**HIGH SENSITIVITY:** if at least two of the control output parameters showed at least ±30% change compared to the identical control parameter of the equivalent ‘base case’, which also significantly affected the general flow pattern, or caused significant changes in the temporal period of temperature oscillation;

**LOW SENSITIVITY:** if at most one of the control output parameters showed a higher change (> ±30%) compared to the identical control parameter of the equivalent ‘base case’, then the general flow pattern and period of temperature oscillation are considered not significantly affected.
For evaluating the effects on the general flow pattern, the number of upwellings, as well as the number of separate flow systems (convection cells) were taken into consideration, and summarised in the corresponding tables.

### 3.4.1 Analyses based on the initial stage of the system

**Model sensitivity to hydraulic properties**

During the simulation of the evolitional stages (Chapter 3.3), the observed hydraulic properties of the carbonate unit (K and η) were slightly increased in the model with respect to published local-scale values to account for regional fracture networks and interconnected karstic channels which would tend to increase the hydraulic properties on the regional scale. Since the scale effect of hydraulic conductivity and porosity in carbonate systems depends strongly on the degree of karstification, as well as on the density of its fracture and conduit network (Király, 1975), effects of lower hydraulic conductivity and porosity on the flow and temperature field were examined. As Jiang et al. (2009) highlighted, development of local versus regional flow systems is sensitive to the rate of decay in K with depth, therefore, a linear decrease of hydraulic conductivity was also tested.

Regarding the low-permeability siliciclastic cover, a higher anisotropy could also be reasonable due to sediment compaction, therefore, the original anisotropy of $K_x/K_z=10$ was increased to $K_x/K_z=100$ by decreasing the vertical hydraulic conductivity ($K_z$) to $10^{-9}$ ms$^{-1}$. The parameters of the simulation scenarios are summarized in Table 3.

As the results showed, the fluid flow pattern and heat distribution are strongly dependent on the hydraulic conductivity of the carbonate. An order of magnitude decrease of K (Case 2) led to the development of weaker steady-state convection cells with a significant ~67% decrease in maximum vertical flow velocity (from $3.1 \times 10^{-7}$ ms$^{-1}$ (Base case) to $7.1 \times 10^{-8}$ ms$^{-1}$) (Table 4). On the other hand, a linear decrease of K (Case 1) resulted in a higher average hydraulic conductivity within the carbonate compare to the Base case, and as a consequence, stronger convection developed (Figure 16b). Both changes of K led to an increase of the maximum attained temperature ($T_{(max)}$) (Table 4). In Case 1, the maximum temperature increased moderately by +13% (from 89.1 °C (Base case) to 100.5 °C), and in parallel, the period and amplitude of temperature oscillations decreased (Figure 17b), while in Case 2 (lower K), $T_{(max)}$ increased by +42% (from 89.1 °C (Base case) to 126.6 °C) (Table 4). Changes in porosity of the carbonate unit had no significant effects on flow velocities and temperature, however, the number of upwellings decreased (from 6 (Base case) to 4), and the convection cells became horizontally elongated.
(Figure 16d, Figure 16e). Higher anisotropy (i.e. lower vertical K) of the cover formation enhanced its insulating role, and led to an increase of average temperature within the carbonate unit (Figure 16f).

Table 3 – Overview of the tested simulation scenarios and the main effects of different hydraulic properties on flow pattern, flow velocities and temperature

<table>
<thead>
<tr>
<th>Case</th>
<th>Parameters</th>
<th>Effects on general flow pattern(1)</th>
<th>Effects on flow dynamics(2)</th>
<th>Effects on temperature field(3)</th>
<th>Overall sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base case: Stage 1</td>
<td>See parameters of Stage 1 in Table 2</td>
<td>*</td>
<td>*</td>
<td>*</td>
<td></td>
</tr>
<tr>
<td>Case 1</td>
<td>Linear decay of K in carbonate from $10^{-7}$ ms$^{-1}$ (top) to $10^{-6}$ ms$^{-1}$ (bottom)</td>
<td>Convection cells also develop close to the base, nr. of upwellings (U6) and nr. of flow systems (S3) remained the same</td>
<td>significantly increased by 99%</td>
<td>significantly increased by 345%</td>
<td>moderately increased by 13%</td>
</tr>
<tr>
<td>Case 2</td>
<td>One order of magnitude lower K of carbonate: exp. decrease from $10^{-5}$ ms$^{-1}$ (top) to $10^{-7}$ ms$^{-1}$ (bottom)</td>
<td>Steady-state convection, less upwellings (U4), more compartmentalized flow field (S4)</td>
<td>significantly decreased by -71%</td>
<td>significantly decreased by -68%</td>
<td>significantly increased by 42%</td>
</tr>
<tr>
<td>Case 3</td>
<td>Uniform 0.2 porosity of carbonate</td>
<td>Shape of the cells is horizontally elongated, less upwellings (U4), less compartmentalized flow field (S2)</td>
<td>significantly increased by 69%</td>
<td>moderately increased by 12%</td>
<td>decreased by -1%</td>
</tr>
<tr>
<td>Case 4</td>
<td>Lower porosity of carbonate (linear decrease from 0.2 (top) to 0.1 (bottom))</td>
<td>No significant effect, less upwellings (U4), nr. of flow systems remained the same (S3)</td>
<td>moderately increased by 27%</td>
<td>significantly increased by 35%</td>
<td>increased by 1%</td>
</tr>
<tr>
<td>Case 5</td>
<td>Higher anisotropy of cover ($K_x/K_z=100$) by decreasing $K_z$ of cover to $10^{-6}$ ms$^{-1}$</td>
<td>Core of the cells are concentrated at the top of the carbonate, less upwellings (U5), more flow systems (S4)</td>
<td>moderately increased by 27%</td>
<td>decreased by -2%</td>
<td>increased by 8%</td>
</tr>
</tbody>
</table>

(1) Figure 16; (2) Table 4; (3) Figure 17, Table 4
U1, U2, etc. represent the number of upwellings; S1, S2, etc. represent the number of flow systems

Table 4 – Maximum horizontal ($V_{x(max)}$) and vertical ($V_{z(max)}$) flow velocity and maximum temperature ($T_{(max)}$) reached over the 220 kyr simulation time resulting from different hydraulic properties

<table>
<thead>
<tr>
<th></th>
<th>Base case (Stage 1)</th>
<th>Case 1 (lin. decay of K)</th>
<th>Case 2 (lower K)</th>
<th>Case 3 (uniform η)</th>
<th>Case 4 (lower η)</th>
<th>Case 5 (higher anisotropy of cover)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_{x(max)}$</td>
<td>$3.5 \times 10^{-7}$ ms$^{-1}$</td>
<td>$6.9 \times 10^{-7}$ ms$^{-1}$</td>
<td>$1.0 \times 10^{-7}$ ms$^{-1}$</td>
<td>$5.8 \times 10^{-7}$ ms$^{-1}$</td>
<td>$4.4 \times 10^{-7}$ ms$^{-1}$</td>
<td>$4.4 \times 10^{-7}$ ms$^{-1}$</td>
</tr>
<tr>
<td>$V_{z(max)}$</td>
<td>$3.1 \times 10^{-7}$ ms$^{-1}$</td>
<td>$1.5 \times 10^{-6}$ ms$^{-1}$</td>
<td>$7.1 \times 10^{-8}$ ms$^{-1}$</td>
<td>$3.5 \times 10^{-7}$ ms$^{-1}$</td>
<td>$4.3 \times 10^{-7}$ ms$^{-1}$</td>
<td>$3.0 \times 10^{-7}$ ms$^{-1}$</td>
</tr>
<tr>
<td>$T_{(max)}$</td>
<td>89.1 °C</td>
<td>100.5 °C</td>
<td>126.6 °C</td>
<td>88.8 °C</td>
<td>89.9 °C</td>
<td>96.0 °C</td>
</tr>
</tbody>
</table>
Figure 16 – Effects of different hydraulic properties on the flow field and temperature distribution after 220 kyr. a) Original Stage 1 (Base case); modified flow field and temperature distribution by b) linear decay of $K$ in carbonate (Case 1); c) lower $K$ of carbonate (Case 2); d) uniform porosity of carbonate (Case 3); e) lower porosity of carbonate (Case 4); f) higher anisotropy of cover (Case 5). M-1, M-2, M-3 and M-4 are locations of monitor points. Values in °C above the sections represent $T_{(\text{max})}$ at 220 kyr. S1, S2, etc. represent the number of flow systems of the different cases. U1, U2, etc. represent the upwellings of the different cases. $Ra$ identifies the location and value of the maximum Rayleigh number within the carbonate unit.
Figure 17 – Effects of different hydraulic properties on temperature oscillations over the 220 kyr simulation time at the monitor points (see Figure 8). a) Original Stage 1 (Base case); modified cyclic temperature oscillation by b) linear decay of $K$ in carbonate (Case 1); c) lower $K$ of carbonate (Case 2); d) uniform porosity of carbonate (Case 3); e) lower porosity of carbonate (Case 4); f) higher anisotropy of cover (Case 5). For Locations of monitor points shown in Figure 16a. Horizontal bars with times (kyr) represent the mean periods of the respective temperature oscillations.
Model sensitivity to thermal conductivity

Thermal conductivity of the carbonate unit was tested based on a realistic interval defined by Luckner and Schestakow (1991), i.e. between 2.0 Wm\(^{-1}\)°C\(^{-1}\) and 3.3 Wm\(^{-1}\)°C\(^{-1}\), with results summarised in Table 5. Although the modified values had only minor effects on the temperature field (Figure 18), as results show, as the thermal conductivity of the carbonate unit increases, the number of upwellings and convection cells decreases, and in parallel, the period of temperature oscillation also decreases to a limited extent (Figure 19).

Table 5 – Overview of the tested simulation scenarios and the main effects of different thermal conductivity of the carbonate unit on flow pattern, flow velocities and temperature

<table>
<thead>
<tr>
<th>Case</th>
<th>Parameters</th>
<th>Effects on general flow pattern(^{(1)})</th>
<th>Effects on flow dynamics(^{(2)})</th>
<th>Effects on temperature field(^{(3)})</th>
<th>Overall sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base case: Stage 1</td>
<td>See parameters of Stage 1 in Table 2</td>
<td>Flow characteristics remained the same, nr. of upwellings increased (U7), more compartmentalized flow field (S4)</td>
<td>significantly increased by 32%</td>
<td>decreased by -9%</td>
<td>increased by 8%</td>
</tr>
<tr>
<td>Case 6</td>
<td>2.0 Wm(^{-1})°C(^{-1}) (min.) thermal conductivity of carbonate</td>
<td>Flow characteristics remained the same, nr. of upwellings increased (U7), more compartmentalized flow field (S4)</td>
<td>significantly increased by 32%</td>
<td>decreased by -9%</td>
<td>increased by 8%</td>
</tr>
<tr>
<td>Case 7</td>
<td>3.3 Wm(^{-1})°C(^{-1}) (max.) thermal conductivity of carbonate</td>
<td>Flow characteristics remained the same, nr. of upwellings decreased (U3), less compartmentalized flow field (S2)</td>
<td>moderately decreased by -10%</td>
<td>moderately decreased by -22%</td>
<td>decreased by -4%</td>
</tr>
</tbody>
</table>

\(^{(1)}\) Figure 18; \(^{(2)}\) Table 6; \(^{(3)}\) Figure 19, Table 6
U1, U2, etc. represent the number of upwellings; S1, S2, etc. represent the number of flow systems

Table 6 – Maximum horizontal \(V_x(max)\) and vertical \(V_z(max)\) flow velocity and maximum temperature \(T_{(max)}\) reached over the 220 kyr simulation time with changes in thermal conductivity of the carbonate unit

<table>
<thead>
<tr>
<th></th>
<th>Base case (Stage 1)</th>
<th>Case 6 (min. thermal K of carbonate)</th>
<th>Case 7 (max. thermal K of carbonate)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(V_x(max))</td>
<td>3.5×10(^{-7}) ms(^{-1})</td>
<td>4.6×10(^{-7}) ms(^{-1})</td>
<td>3.1×10(^{-7}) ms(^{-1})</td>
</tr>
<tr>
<td>(V_z(max))</td>
<td>3.1×10(^{-7}) ms(^{-1})</td>
<td>2.8×10(^{-7}) ms(^{-1})</td>
<td>2.3×10(^{-7}) ms(^{-1})</td>
</tr>
<tr>
<td>(T_{(max)})</td>
<td>89.1 °C</td>
<td>96.5 °C</td>
<td>85.4 °C</td>
</tr>
</tbody>
</table>
Figure 18 – Effects of different thermal conductivity of the carbonate unit on the flow field and temperature distribution after 220 kyr. a) Original Stage 1 (Base case); modified flow field and temperature distribution by using b) minimum thermal conductivity of carbonates (Case 6); c) maximum thermal conductivity of carbonates (Case 7). M-1, M-2, M-3 and M-4 are locations of monitor points. Values in °C above the sections represent $T_{\text{max}}$ at 220 kyr. S1, S2, etc. represent the number of flow systems of the different cases. U1, U2, etc. represent the upwellings of the different cases. Ra identifies the location and value of the maximum Rayleigh number within the carbonate unit.
Figure 19 – Effects of different thermal conductivity of the carbonate unit on temperature oscillations over the 220 kyr simulation time at the monitor points (see Figure 18a). a) Original Stage 1 (Base case); modified cyclic temperature oscillation by using b) a minimum thermal conductivity of carbonates (Case 6); c) a maximum thermal conductivity of carbonates (Case 7). Horizontal bars with times (kyr) represent the mean periods of the respective temperature oscillations.
Model sensitivity to geological conditions

Since verification of the conceptual model in the early evolutionary stages of the BTK system was not possible due to the lack of direct data, the effects of key parameters regarding the geological conditions on flow the field and heat distribution were evaluated herein (Table 7).

Originally, the 800 m thickness of the cover formation above the carbonate (during Stage 1, used as the Base case) was estimated based on the fluid inclusion study of Poros et al. (2012). Therefore, effects of a thicker (1200 m) and thinner (400 m) cover above the 3200 m thick carbonate formation were tested. To facilitate comparisons among the different simulated geological evolutionary stages of the system, a uniform heat flux of 100 mWm$^{-2}$ was defined in all stages during investigation of fluid flow evolution on geological time scales. However, based on the work of Balázs et al. (2017), the heat flux below the pilot area could have been higher, up to approx. 120 mWm$^{-2}$ due to the extension of the Pannonian Basin (which has exponentially decreased to the current value of 100 mWm$^{-2}$). This higher heat flux, as a possible value in this evolutionary stage, was therefore also tested as part of the sensitivity analysis.

Increased thickness of the cover (Case 8) led to an increase of average temperature within the carbonate due to its improved insulation effect (Figure 20b), and led to a significant increase of maximum flow velocities (+60% increase of $V_{x\text{max}}$ and +20% increase of $V_{z\text{max}}$) (Table 8). A lower period of temperature oscillations also reflects a more dynamic system compared to the Base case (Figure 21b). On the other hand, in Case 9 with a thinner cover, steady-state convection cells created a more compartmentalized temperature field within the carbonate unit at 220 kyr (Figure 20c).

Results also showed that a 20% increase in heat flux caused an approx. +40% change in maximum flow velocities (Case 10 in Table 8) and a +10% increase in maximum temperature, although the main characteristics of the convection-dominated flow system remained the same.
CHAPTER 3

NUMERICAL INVESTIGATIONS

Table 7 – Overview of the tested simulation scenarios and the main effects of different geological conditions on flow pattern, flow velocities and temperature

<table>
<thead>
<tr>
<th>Case</th>
<th>Parameters</th>
<th>Effects on general flow pattern(1)</th>
<th>Effects on flow dynamics(2)</th>
<th>Effects on temperature field(3)</th>
<th>Overall sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base case: Stage 1</td>
<td>Parameters of Stage 1 in Table 2</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Case 8</td>
<td>Thicker (1200 m) cover above the 3200 m thick carbonate</td>
<td>Flow characteristics and nr. of upwellings (U6) remained the same, more compartmentalized flow field (S4)</td>
<td>significantly increased by 62%</td>
<td>moderately increased by 17%</td>
<td>increased by 7%</td>
</tr>
<tr>
<td>Case 9</td>
<td>Thinner (400 m) cover above the 3200 m thick carbonate</td>
<td>Steady-state convection with less upwellings (U4), more compartmentalized flow field (S4)</td>
<td>significantly decreased by 45%</td>
<td>significantly decreased by 47%</td>
<td>decreased by 8%</td>
</tr>
<tr>
<td>Case 10</td>
<td>120 mWm$^{-2}$ heat flux along the bottom</td>
<td>Flow characteristics remained the same, nr. of upwellings decreased (U5), nr. of flow systems remained the same (S3)</td>
<td>significantly decreased by 48%</td>
<td>significantly increased by 38%</td>
<td>increased by 10%</td>
</tr>
</tbody>
</table>

(1) Figure 20; (2) Table 8; (3) Figure 21, Table 8
U1, U2, etc. represent the number of upwellings; S1, S2, etc. represent the number of flow systems

Table 8 – Maximum horizontal ($V_{x(\text{max})}$) and vertical ($V_{z(\text{max})}$) flow velocity and maximum temperature ($T_{(\text{max})}$) reached over the 220 kyr simulation time with changes in geological conditions

<table>
<thead>
<tr>
<th></th>
<th>Base case (Stage 1)</th>
<th>Case 8 (thicker cover)</th>
<th>Case 9 (thinner cover)</th>
<th>Case 10 (higher heatflux)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_{x(\text{max})}$</td>
<td>3.5×10^{-7} ms$^{-1}$</td>
<td>5.6×10^{-7} ms$^{-1}$</td>
<td>1.9×10^{-7} ms$^{-1}$</td>
<td>5.1×10^{-7} ms$^{-1}$</td>
</tr>
<tr>
<td>$V_{z(\text{max})}$</td>
<td>3.1×10^{-7} ms$^{-1}$</td>
<td>3.7×10^{-7} ms$^{-1}$</td>
<td>1.5×10^{-7} ms$^{-1}$</td>
<td>4.4×10^{-7} ms$^{-1}$</td>
</tr>
<tr>
<td>$T_{(\text{max})}$</td>
<td>89.1 °C</td>
<td>95.5 °C</td>
<td>81.7 °C</td>
<td>98.4 °C</td>
</tr>
</tbody>
</table>
Figure 20 – Effects of geological conditions on flow field and temperature distribution after 220 kyr. a) Original Stage 1 (Base case); modified flow field and temperature distribution resulting from b) a thicker (1200 m) cover above the carbonate (Case 8); c) a thinner (400 m) cover above the carbonate (Case 9); d) a higher (120 mWm$^{-2}$) basal heat flux (Case 10). M-1, M-2, M-3 and M-4 are locations of monitor points. Values in °C above the sections represent $T_{\text{max}}$ at 220 kyr. S1, S2, etc. represent the number of flow systems of the different cases. U1, U2, etc. represent the upwellings of the different cases. Ra identifies the location and value of the maximum Rayleigh number within the carbonate unit.
Figure 21 – Effects of different geological conditions on temperature oscillations over the 220 kyr simulation time at the monitor points (see Figure 20a). a) Original Stage 1 (Base case); modified cyclic temperature oscillation resulting from b) a thicker (1200 m) cover above the carbonate (Case 8); c) a thinner (400 m) cover above the carbonate (Case 9); d) a higher (120 mWm$^{-2}$) basal heat flux (Case 10). Horizontal bars with times (kyr) represent the mean periods of the respective temperature oscillations.
3.4.2 Analyses based on the recent (current) state of the system

Model sensitivity to hydraulic properties

In the sensitivity study of Stage 4, the same hydraulic properties were tested (summarised in Table 9) as in the case of Stage 1. Based on the results of the simulations, significant changes in temperature were caused only by the changes in hydraulic conductivity. In Case 1 (linear decay of K), a higher average K in the carbonate led to a −21% decrease in $T_{\text{max}}$ with no notable effects on flow velocities, while in Case 2 (an order of magnitude lower K), $T_{\text{max}}$ increased by +71% (from 88.3 °C (Base case) to 150.6 °C) in parallel with a significant decrease of flow velocities (Table 10). A decrease in porosity led to an increase of flow velocity ($V_{x(\text{max})}$ increased by +51%, while $V_{z(\text{max})}$ increased by +39% compared to the Base case), however, it caused no significant effects on flow field and heat distribution (Table 10). With conditions of Case 2 (lower K) and Case 5 (higher anisotropy of cover), groundwater contribution from the cover formation to the carbonate unit is restricted (Figure 22b, Figure 22f). Moreover, flow direction within the cover reversed in Case 2 (Figure 22c).
Table 9 – Overview of the tested simulation scenarios and the main effects of different hydraulic properties on flow pattern, flow velocities and temperature

<table>
<thead>
<tr>
<th>Case</th>
<th>Parameters</th>
<th>Effects on general flow pattern(1)</th>
<th>Effects on flow dynamics(2)</th>
<th>Effects on temperature field(3)</th>
<th>Overall sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base case: Stage 4</td>
<td>See parameters of Stage 4 in Table 2</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Case 1</td>
<td>Linear decay of K in carbonate from $10^{-4}$ ms$^{-1}$ (top) to $10^{-6}$ ms$^{-1}$ (bottom)</td>
<td>Flow characteristics remained the same, nr. of upwellings decreased (U3), nr. of flow systems remained the same (S3)</td>
<td>increased by 5%</td>
<td>increased by 1%</td>
<td>moderately decreased by -21%</td>
</tr>
<tr>
<td>Case 2</td>
<td>One order of magnitude lower K of carbonate: exp. decrease from $10^{-5}$ ms$^{-1}$ (top) to $10^{-7}$ ms$^{-1}$ (bottom)</td>
<td>Upward flow within the entire cover, nr. of upwellings (U2) and nr. of flow systems (S2) also decreased</td>
<td>significantly decreased by -85%</td>
<td>significantly decreased by -70%</td>
<td>significantly increased by 71%</td>
</tr>
<tr>
<td>Case 3</td>
<td>Uniform 0.2 porosity of carbonate</td>
<td>Flow characteristics remained the same, nr. of upwellings decreased (U3), nr. of flow systems remained the same (S3)</td>
<td>significantly increased by 49%</td>
<td>significantly increased by 34%</td>
<td>decreased by -1%</td>
</tr>
<tr>
<td>Case 4</td>
<td>Lower porosity of carbonate: linear decrease from 0.2 (top) to 0.1 (bottom)</td>
<td>Flow characteristics remained the same, nr. of upwellings decreased (U3), nr. of flow systems remained the same (S3)</td>
<td>significantly increased by 49%</td>
<td>moderately increased by 29%</td>
<td>decreased by -2%</td>
</tr>
<tr>
<td>Case 5</td>
<td>Higher anisotropy of cover ($K_x/K_z=100$) by decreasing $K_z$ of cover to $10^{-9}$ ms$^{-1}$</td>
<td>Flow within the cover is mainly horizontal, nr. of upwellings decreased (U3), nr. of flow systems remained the same (S3)</td>
<td>no change</td>
<td>decreased by -1%</td>
<td>decreased by -1%</td>
</tr>
</tbody>
</table>

(1) Figure 22; (2) Table 10; (3) Figure 23, Table 10
U1, U2, etc. represent the number of upwellings; S1, S2, etc. represent the number of flow systems

Table 10 – Maximum horizontal ($V_{x(max)}$) and vertical ($V_{z(max)}$) flow velocity and maximum temperature ($T_{(max)}$) reached over the 220 kyr simulation time with changes in hydraulic properties

<table>
<thead>
<tr>
<th></th>
<th>Base case (Stage 4)</th>
<th>Case 1 (lin. decay of K)</th>
<th>Case 2 (lower K)</th>
<th>Case 3 (uniform η)</th>
<th>Case 4 (lower η)</th>
<th>Case 5 (higher anisotropy of cover)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_{x(max)}$</td>
<td>$9.3 \times 10^{-7}$ ms$^{-1}$</td>
<td>$9.8 \times 10^{-7}$ ms$^{-1}$</td>
<td>$1.4 \times 10^{-7}$ ms$^{-1}$</td>
<td>$1.4 \times 10^{-6}$ ms$^{-1}$</td>
<td>$1.4 \times 10^{-6}$ ms$^{-1}$</td>
<td>$9.3 \times 10^{-7}$ ms$^{-1}$</td>
</tr>
<tr>
<td>$V_{z(max)}$</td>
<td>$7.9 \times 10^{-7}$ ms$^{-1}$</td>
<td>$8.0 \times 10^{-7}$ ms$^{-1}$</td>
<td>$1.4 \times 10^{-7}$ ms$^{-1}$</td>
<td>$1.1 \times 10^{-6}$ ms$^{-1}$</td>
<td>$1.1 \times 10^{-6}$ ms$^{-1}$</td>
<td>$7.9 \times 10^{-7}$ ms$^{-1}$</td>
</tr>
<tr>
<td>$T_{(max)}$</td>
<td>88.3 °C</td>
<td>70.1 °C</td>
<td>150.6 °C</td>
<td>88.2 °C</td>
<td>86.6 °C</td>
<td>87.9 °C</td>
</tr>
</tbody>
</table>
Figure 22 – Effects of different hydraulic properties on the flow field and temperature distribution after 220 kyr. a) Original Stage 4 (Base case); modified flow field and temperature distribution resulting from b) a linear decay of K in carbonate (Case 1); c) a lower K of carbonate (Case 2); d) a uniform porosity of carbonate (Case 3); e) a lower porosity of carbonate (Case 4); f) higher anisotropy of the cover (Case 5). M-1, M-2, M-3 and M-4 are locations of monitor points. Values in °C above the sections represent $T_{\text{max}}$ at 220 kyr. S1, S2, etc. represent the number of flow systems of the different cases. U1, U2, etc. represent the upwellings of the different cases. Ra identifies the location and value of the maximum Rayleigh number within the carbonate unit.
Figure 23 – Effects of different hydraulic properties on temperature oscillations over the 220 kyr simulation time at the monitor points (see Figure 22a). a) Original Stage 4 (Base case); modified cyclic temperature oscillation resulting from b) a linear decay of $K$ in carbonate (Case 1); c) a lower $K$ of carbonate (Case 2); d) a uniform porosity of carbonate (Case 3); e) a lower porosity of carbonate (Case 4); f) a higher anisotropy of the cover (Case 5). The first 40 kyr of the simulation were excluded from the analysis due to initial instabilities. Horizontal bars with times (kyr) represent the mean periods of the respective temperature oscillations.
Model sensitivity to geological conditions

Across the bottom boundary, a heat flux of 100 mWm\(^{-2}\), characteristic for the analogue pilot area, was defined in the current stage of the system (Stage 4) based on Lenkey et al. (2002). In order to evaluate the effect of basal heat flux on the flow field and temperature distribution within the partly confined carbonate system, a 60 mWm\(^{-2}\) global average heat flux, and a 85 mWm\(^{-2}\) average heat flux typical of extensional basins (Allen and Allen, 2013) were also tested (Table 11).

With the lowest applied heat flux (Case 6, 60 mWm\(^{-2}\)), steady-state conditions were reached rapidly (Figure 25b). In the case of applying an average heat flux of extensional basins (Case 7), an approx. 15 kyr period of temperature oscillation is characteristic, similar to the Base case (Figure 25c). None of the modifications to the heat flux significantly affected the flow velocities (Table 12). However, a linear relationship between the heat flux, number of upwellings (Figure 24) and maximum reached temperature (Table 12) was found. A decrease of heat flux by ~40% resulted in a decrease of temperature by ~17% in Case 6 compared to the Base case, while a decrease of heat flux by ~15% resulted in a decrease of temperature by ~6% in Case 7 (Table 12).

<table>
<thead>
<tr>
<th>Case</th>
<th>Parameters</th>
<th>Effects on general flow pattern(1)</th>
<th>Effects on flow dynamics(2)</th>
<th>Effects on temperature field(3)</th>
<th>Overall sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base case: Stage 4</td>
<td>See parameters of Stage 4 in Table 2</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Case 6</td>
<td>60 mWm(^{-2}) global average heatflux</td>
<td>Flow characteristics and nr. of flow systems (S3) remained the same, nr. of upwellings decreased (U2)</td>
<td>no change</td>
<td>moderately decreased by -17%</td>
<td>low</td>
</tr>
<tr>
<td>Case 7</td>
<td>85 mWm(^{-2}) average heatflux of extensional basins</td>
<td>Flow characteristics and nr. of flow systems (S3) remained the same, nr. of upwellings decreased (U3)</td>
<td>no change</td>
<td>decreased by -10%</td>
<td>low</td>
</tr>
</tbody>
</table>

(1) Figure 24; (2) Table 12; (3) Figure 25, Table 12
U1, U2, etc. represent the number of upwellings; S1, S2, etc. represent the number of flow systems

Table 12 – Maximum horizontal \(V_{x{(\text{max})}}\) and vertical \(V_{z{(\text{max})}}\) flow velocity and maximum temperature \(T_{(\text{max})}\) reached over the 220 kyr simulation time with changes in basal heat flux

<table>
<thead>
<tr>
<th></th>
<th>Base case (Stage 4)</th>
<th>Case 8 (lower water table slope)</th>
<th>Case 9 (higher water table slope)</th>
<th>Case 10 (cosine water table slope)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(V_{x{(\text{max})}})</td>
<td>9.3×10^{-7} ms(^{-1})</td>
<td>7.4×10^{-7} ms(^{-1})</td>
<td>1.2×10^{-6} ms(^{-1})</td>
<td>1.3×10^{-6} ms(^{-1})</td>
</tr>
<tr>
<td>(V_{z{(\text{max})}})</td>
<td>7.9×10^{-7} ms(^{-1})</td>
<td>8.2×10^{-7} ms(^{-1})</td>
<td>8.5×10^{-7} ms(^{-1})</td>
<td>8.2×10^{-7} ms(^{-1})</td>
</tr>
<tr>
<td>(T_{(\text{max})})</td>
<td>88.3 °C</td>
<td>88.2 °C</td>
<td>88.8 °C</td>
<td>84.8 °C</td>
</tr>
</tbody>
</table>
Figure 24 – Effects of the different basal heat fluxes on the flow field and temperature distribution after 220 kyr.

a) Original Stage 4 (Base case); modified flow field and temperature distribution resulting from b) a 60 mW m$^{-2}$ world average heat flux (Case 6); c) a 85 mW m$^{-2}$ average heat flux of extension basins (Case 7). M-1, M-2, M-3 and M-4 are locations of monitor points. Values in °C above the sections represent $T_{\text{max}}$ at 220 kyr. S1, S2, etc. represent the number of flow systems of the different cases. U1, U2, etc. represent the upwellings of the different cases. Ra indicates the location and value of the maximum Rayleigh number within the carbonate unit.
Figure 25 – Effects of different basal heat fluxes on temperature oscillations over the 220 kyr simulation time at the monitor points (see Figure 24a). a) Original Stage 4 (Base case); modified cyclic temperature oscillation resulting from b) 60 mWm$^{-2}$ global average heat flux (Case 6); c) 85 mWm$^{-2}$ average heat flux of extension basins (Case 7). Horizontal bars with times (kyr) represent the mean periods of the respective temperature oscillations.
Model sensitivity to the slope of the water table

Since the regional slope and shape of the water table is a critical factor in shaping the flow system, different water table slopes and shapes were also tested for the unconfined carbonate subsystem. The water table along the covered sub-system remains unchanged (Table 13) in order to eliminate ensemble effects of modified slopes along both sub-systems.

A lower slope of the water table (Case 8) led to an increased period of temperature oscillation (from 15 kyr (Base case) to 20 kyr), while a higher slope of the water table (Case 9) increased the amplitude of the cyclic temperature oscillations (from approx. 22 °C (Base case) to 30 °C) (Figure 27). Maximum vertical flow remained unchanged, however maximum horizontal flow was altered significantly by each modification (by –20%, +29% and +40% in Case 8, Case 9 and Case 10; Table 14). Maximum temperatures remained unaffected in all cases (Table 14).

Although the main characteristics of the flow field and heat distribution remained unchanged, upwellings from the bottom of the carbonate shifted toward the west, caused by a lower slope in Case 8 (Figure 26b). On the other hand, a higher slope (Case 9) caused a shift of convection cells toward east (Figure 26c). A cosine water table slope led to the development of two distinct discharge zones within the west sub-basin (Figure 26d) with low (<15°C) discharging temperatures.
Table 13 – Overview of the tested simulation scenarios and the main effects of different water table slopes on flow pattern, flow velocities and temperature

<table>
<thead>
<tr>
<th>Case</th>
<th>Parameters</th>
<th>Effects on general flow pattern(1)</th>
<th>Effects on flow dynamics(2)</th>
<th>Effects on temperature field(3)</th>
<th>Overall sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base case: Stage 4</td>
<td>See parameters of Stage 4 in Table 2</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Case 8</td>
<td>Lower (-30%) slope of water table along the W subsystem (hydraulic head at the W boundary decreased from 31 m to 21.7 m)</td>
<td>Upwellings shifted toward west, nr. of upwellings (U4) and nr. of flow systems (S3) remained the same</td>
<td>moderately decreased by -20%</td>
<td>increased by 4%</td>
<td>decreased by -1%</td>
</tr>
<tr>
<td>Case 9</td>
<td>Higher (+30%) slope of water table along the W subsystem (hydraulic head at the W boundary increased from 31 m to 40.3 m)</td>
<td>Upwellings shifted toward east, nr. of upwellings (U4) and nr. of flow systems (S3) remained the same</td>
<td>significantly increased by 30%</td>
<td>increased by 6%</td>
<td>increased by 1%</td>
</tr>
<tr>
<td>Case 10</td>
<td>Cosine water table along the W subsystem (1.5 cosine cycle with an amplitude of 2 m)</td>
<td>Local discharge zone appears within the uncovered sub-system, nr. of upwellings decreased (U3), more compartmentalized flow system (S5)</td>
<td>significantly increased by 42%</td>
<td>increased by 3%</td>
<td>decreased by -4%</td>
</tr>
</tbody>
</table>

(1) Figure 26; (2) Table 14; (3) Figure 27, Table 14
U1, U2, etc. represent the number of upwellings; S1, S2, etc. represent the number of flow systems

Table 14 – Maximum horizontal ($V_{x(max)}$) and vertical ($V_{z(max)}$) flow velocity and maximum temperature ($T_{(max)}$) reached over the 220 kyr simulation time with changes in water table slope

<table>
<thead>
<tr>
<th>Case</th>
<th>$V_{x(max)}$</th>
<th>$V_{z(max)}$</th>
<th>$T_{(max)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base case (Stage 4)</td>
<td>9.3×10^{-7} ms^{-1}</td>
<td>7.9×10^{-7} ms^{-1}</td>
<td>88.3 °C</td>
</tr>
<tr>
<td>Case 1 (lower water table slope)</td>
<td>7.4×10^{-7} ms^{-1}</td>
<td>8.2×10^{-7} ms^{-1}</td>
<td>88.2 °C</td>
</tr>
<tr>
<td>Case 2 (higher water table slope)</td>
<td>1.2×10^{-6} ms^{-1}</td>
<td>8.5×10^{-7} ms^{-1}</td>
<td>88.8 °C</td>
</tr>
<tr>
<td>Case 3 (cosine water table slope)</td>
<td>1.3×10^{-5} ms^{-1}</td>
<td>8.2×10^{-7} ms^{-1}</td>
<td>84.8 °C</td>
</tr>
</tbody>
</table>
Figure 26 - Effects of different water table slopes on the flow field and temperature distribution after 220 kyr. 

a) Original Stage 4 (Base case); modified flow field and temperature distribution resulting from b) a lower water table slope of the W subsystem (Case 8); c) a higher water table slope of the W subsystem (Case 9); d) a cosine water table slope of the W subsystem (Case 10). M-1, M-2, M-3 and M-4 are locations of monitor points. Values in °C above the sections represent $T_{\text{max}}$ at 220 kyr. S1, S2, etc. represent the number of flow systems of the different cases. U1, U2, etc. represent the upwellings of the different cases. Ra identifies the location and value of the maximum Rayleigh number within the carbonate unit.
Figure 27 – Effects of different water table slopes on temperature oscillations over the 220 kyr simulation time at the monitor points (see Figure 26a). a) Original Stage 4 (Base case); modified cyclic temperature oscillation resulting from b) a lower water table slope of the W subsystem (Case 8); c) a higher water table slope of the W subsystem (Case 9); d) a cosine water table slope of the W subsystem (Case 10). Horizontal bars with times (kyr) represent the mean periods of the respective temperature oscillations.
3.4.3 Interpretation and discussion

Deviations in maximum temperature and flow velocities caused by the modified parameters were compared to the otherwise identical base case simulation for each stage in order to evaluate their relative importance on flow dynamics and consequent temperature distribution. Because the coupled system is thermally unstable, in which convection cells regularly develop and disappear over time, comparisons were made based on the maximum flow velocities ($V_{x(\text{max})}$ and $V_{z(\text{max})}$), and maximum temperature ($T_{(\text{max})}$) reached over the entire 220 kyr simulation time interval.

The maximum temperature of Stage 1 was affected by the selected key parameters to a relatively limited extent, with changes in $T_{(\text{max})}$ remaining below 10% in most cases except those which caused by modification of hydraulic conductivity values (Figure 28). In Stage 4, the change of $T_{(\text{max})}$ was even smaller, below 5%, except for changes caused by the hydraulic conductivity (Figure 29). In the initial state of the system (Stage 1), an order of magnitude decrease of hydraulic conductivity led to an increase of the maximum temperature by +42%, while in the partly unconfined current state of the system (Stage 4), $T_{(\text{max})}$ changed by +71%. The significant difference between induced changes in $T_{(\text{max})}$ of these stages can be attributed to changes in the velocity within the partly unconfined system compared to the fully confined case (Figure 30, Figure 31), which result from the gradual change of meteoric water recharge during the system evolution. Compared to the fully confined system (Figure 31), both horizontal and vertical maximum flow velocities were more sensitive in the partly unconfined system (Stage 4) to an order of magnitude decrease in hydraulic conductivity. The velocities in the partly confined system therefore decreased to a greater extent compared to the fully confined system with the decrease in hydraulic conductivity (Figure 31). As a consequence, lower flow velocities provided more efficient heating of groundwater at the bottom of the system, which therefore reached higher temperatures, in agreement with the findings of An et al. (2015).

Development of porosity and hydraulic conductivity in carbonate systems can be affected by the changes in flow patterns and heat distribution over long time scales. An important remaining question is how do changes in hydrogeological system parameters provide feedback to the groundwater flow processes? As the sensitivity study showed, changes in these key input parameters led to significant changes (>30% change) in flow velocity, while induced changes in fluid dynamics caused minor modification in the overall flow and temperature field along the studied section (Figure 16, Figure 22). Therefore, upscaling of the measured local (borehole) scale hydraulic properties of the carbonate (especially hydraulic conductivity) to regional (basin) scale values requires great care.
The magnitude and depth-decay of hydraulic conductivity within the carbonate unit has the most significant effects on flow dynamics and temperatures in both (initial and recent) tested stages. The main character of the flow system remained the same in all tested scenarios of Stage 1, suggesting lower sensitivity. Stage 4 showed higher sensitivity i) to the magnitude of K, which caused upward flow within the cover, and ii) to the cosine water table, which led to a more compartmentalized flow field by the development of local discharge areas. However, in the carbonate system with a well-developed upper karstified zone, the water table is dominantly recharge-controlled (Goderniaux et al., 2013) (Figure 6c), and therefore, water table mounding is reduced.
Figure 30 – Changes in maximum flow velocities of Stage 1 ($V_{x,\text{max}}=3.5\times10^{-7}\ \text{ms}^{-1}$; $V_{z,\text{max}}=3.1\times10^{-7}\ \text{ms}^{-1}$) over the 220 kyr simulation caused by the imposed changes in selected parameters.

Figure 31 – Changes in maximum flow velocities of Stage 4 ($V_{x,\text{max}}=9.3\times10^{-7}\ \text{ms}^{-1}$; $V_{z,\text{max}}=7.9\times10^{-7}\ \text{ms}^{-1}$) over the 220 kyr simulation caused by imposed changes in selected parameters.
3.5 Comparison of the results with characteristics of the pilot area and open questions

Although the simplified semi-synthetic model scenarios focus on regional scale fluid flow and heat transport processes, results can also be discussed with respect to previously investigated site-specific characteristics of the BTK. Moreover, such comparison of the results with site-specific characteristics could serve as verification, since validation of simulation results is strongly limited due to the lack of direct data from the geological past.

In the fully confined initial system state (Stage 1), the flow and temperature field is clearly dominated by natural thermal convection, with maximum temperatures reaching 85 °C, which is consistent with the independently-estimated fluid inclusion temperatures for this stage (Poros et al., 2012). In agreement with the regional distribution of vein-filling minerals and connected paragenesis described by Poros (2011), a uniform groundwater flow system can be assumed within the BTK until the start of uplift in the Late Miocene. Based on the results of previous studies, development of the current porosity of the BTK was assumed to start in Miocene times (Poros, 2011). Porosity and permeability enhancement in that buoyancy-dominated stage may be linked to the increasing dissolution capacity of cooler water raised by convection cells (Andre and Rajaram, 2005; Dublyansky, 2000; Mádl-Szőnyi et al., 2018). Indeed, retrograde solubility of calcite is known to sustain dissolution along a flow path with decreasing temperature, as discussed e.g. by Palmer (1991). This fully confined system is sensitive to changes in hydraulic conductivity, which led to major changes in flow dynamics, however these changes had only minor effects on the flow field and temperature distribution of the system.

Initially, the pore space was assumed to be filled with antecedent seawater (Mádl-Szőnyi et al. 2018). As the area became subaerially exposed, and uplift of the western part of the system began, meteoric water started to infiltrate and dilute the original pore water, and modified the redox conditions within the system, in agreement with vein-filling paragenesis which reflects a more oxidative environment during system evolution (Poros et al. 2012).

Due to uplift, travertines started to form at the margin of the uplifted blocks (Kele et al., 2011; Scheuer and Schweitzer, 1988). As Kele et al. (2011) highlighted, travertines of the Buda Hills precipitated from warmer water (with temperatures between 20 and 65 °C) compared to modern water temperatures (between 20 and 28 °C), which is confirmed by the gradually decreasing temperature of the different simulated stages in parallel with the increase of hydraulic head differences along the groundwater table and decreasing cover thicknesses along the west part.

After 4 Ma, due to the initiated uplift of the eastern sub-system (Ruszkiczyz-Rüdiger et al., 2007), basinal fluid flow toward the main discharge point (along the Danube) began, which could have
contributed to the formation of hypogene caves (Dublyansky et al., 2014; Poros et al., 2012). Such cave formation would not only be due to the mixing of different fluids (Gray and Engel, 2013; Mádl-Szőnyi and Tóth, 2015) but also due to the dissolution-enhancing effect of aggressive gases (e.g. CO$_2$ and H$_2$S) (Palmer, 2007) transported by groundwater from the covered sub-basin (Erőss et al., 2012a; Poros et al., 2012). Although the groundwater geochemistry was neglected in the recent transport modelling, the simulation results confirmed the discharge of water from different flow systems at the boundary of the unconfined and confined carbonate. In particular, flow system S1 is fed by meteoric water across the carbonate, while regional flow system S2 is fed by regional groundwater flow across the west boundary (Figure 11).

Based on the recent (modern) condition and processes of the BTK, Mádl-Szőnyi and Tóth (2015) presented a conceptual model of a carbonate basin at the margin of unconfined and confined sub-systems, in which an interface evolves between fresh meteoric water (originating from an unconfined sub-basin) and chloride-rich basinal fluids (originating from a confined sub-basin), which could represent a potential dissolution zone for porosity enhancement due to the chemical differences between these waters. The simulations presented here show, in addition, the evolution of the recent flow and heat patterns within a geological time frame, and highlight that i) the boundary between these two flow components (designated by stagnation point SP, see Figure 9 and Figure 10) gradually shifted toward the main discharge point of the system (at 15 km) during the geological evolution, and therefore that ii) direct discharge of basinal fluids from the eastern confining layers to the BTK allowed only in recent times.

The results of regional-scale groundwater flow simulations can provide a suitable background to clarify detailed site-specific mass and heat transfer related questions, such as the following examples.

i) How could groundwater flow affect the properties of the carbonate range through long time scales and how will these properties provide feedback to the groundwater flow processes?

ii) What is the interrelationship between paleo-hydrogeological evolution of the BTK and hypogene cave formation?

iii) How could large-scale changes in flow affect the residence time of groundwater in the different parts of the system?

iv) How long does it take to leach brine water from the pores of the low permeable siliciclastic cover of the eastern sub-system?
4 SUMMARY AND CONCLUSIONS

Numerical investigations have provided new insights into the processes controlling fluid flow and heat transport at the margin of unconfined and confined carbonates during their geological evolution. The simulations covered the range from fully confined conditions to the development of unconfined conditions. The Buda Thermal Karst (BTK) of Hungary was used as an analogue pilot area on which to base realistic geological evolutionary stages and physical system parameters. Since the main goal was to gain insight into the effect of decreasing thickness of the low-permeability confining layer on the flow field and heat distribution, a simplified geological and hydrostratigraphic conceptual model was applied. Four scenarios of semi-synthetic models were tested to represent characteristic snapshots of the fluid evolution of the studied system. Moreover, the sensitivity of applied parameters was examined within realistic uncertainty bounds for the initial (Stage 1) and recent (Stage 4) scenarios.

Differential tectonic uplift led to large-scale changes in the importance of different fluid driving forces during system evolution. The following conclusions can be drawn from the numerical experiment on paleohydrogeology and thermal history of marginal confined and unconfined carbonate system.

Characteristics of subsurface fluid flow and heat transport processes at the margin of confined and unconfined carbonate systems with decreasing cover thickness at one ridge

1. As the results of the simulations showed, the flow and temperature fields are clearly dominated by natural thermal convection in the fully confined, initial system state (Stage 1). Transient convection cells with 6-8 concurrent cells gradually dissipate with time while new ones are born, eventually reaching a quasi steady-state pattern with temporally repeating similar patterns (Figure 32a). This vigorous, dynamic system with a maximum groundwater flow velocity of $V_{x\text{max}} = 1.9 \times 10^{-7}$ ms$^{-1}$, is maintained due to the heat insulating role of the low-conductivity siliciclastic confining formation, in which a maximum temperature of 89.1°C at the bottom of the carbonate unit is reached over the 220 kyr simulation time. Porosity enhancement in this buoyancy-dominated stage may be related to the increasing dissolution capacity of cooling water raised by convection cells. The sensitivity study showed that changes in key hydraulic input parameters (hydraulic conductivity, porosity) led to significant changes (>30%) in flow velocities. However, induced changes in fluid dynamics caused only minor modification of the general flow and temperature field along the studied
section. In the BTK pilot area, it can be assumed that this convection-dominated flow system existed before 10 Myr, prior to the start of differential tectonic uplift of the broader area.

2. As revealed by significantly changed flow patterns generated by coupled gravity and buoyant flow compared to pure gravity-driven flow, groundwater movement in Stage 2 and 3 (Figure 32b, c) – characterised by reduced cover thickness at the west sub-system – was still convection-dominated. However, due to the evolved topographic and hydraulic gradient by tectonic uplift, convection cells shifted slightly within the carbonate towards the eastern, confined part of the system. The maximum flow velocity gradually increased during system evolution ($V_{z(\text{max})}$ increased from $1.9\times10^{-7}$ ms$^{-1}$ (Stage 1) to $5.2\times10^{-7}$ ms$^{-1}$ (Stage 3), $V_{x(\text{max})}$ increased from $7.3\times10^{-8}$ ms$^{-1}$ in Stage 1 to $2.3\times10^{-7}$ ms$^{-1}$ in Stage 3).

3. It was performed by the simulations, that cooling of the system significantly progressed to Stage 4 (representing the recent state of the system) (Figure 32d). Because of the relatively high penetration depth (>3000 m) of cold meteoric water within the unconfined carbonate sub-system, groundwater cannot heat up within that part of the system. Water temperature remains at 10-15°C within a substantial part of the unconfined sub-system (to approx. 3000 m depth), in spite of the relatively high basal heat flux (100 mWm$^{-2}$) below the area. Despite the cooling effect of more intensive meteoric infiltration along the west block, a heat accumulation developed within the eastern, covered carbonate sub-system (Figure 32). As previous studies (e.g. Kovács and Müller, 1980; Mádl-Szőnyi and Tóth, 2015) also highlighted, the heat content of discharging groundwater at the margin of the confined and unconfined carbonate parts originates from the covered sub-system. Results of the current study show, in addition, that the asymmetric flow pattern and the boundary between two different flow components (designated by stagnation point SP between S1 and S2 flow systems, see Figure 9 and Figure 10) gradually shifted toward the main discharge point of the system (at 15 km) during the geological evolution.

4. As the results of the simulations showed, discharge patterns changed significantly during the system evolution. Extension of the groundwater discharge zone, developed as tectonic uplift initiated, gradually decreased from 17 km (Stage 2) to 15 km (Stage 3) and 13 km (Stage 4). As system boundaries developed (Stage 3), two separate recharge areas evolved, which led to the compartmentalization of the discharge area. It was performed, that the flow field was significantly modified by further uplift, and led to direct discharge of regional flow at the boundary of the confined and unconfined sub-systems, where the Darcy flux of discharging groundwater significantly increases with time by approx. 3 orders of magnitude from $1.4\times10^{-10}$ ms$^{-1}$ (Stage 2) to $1.8\times10^{-7}$ ms$^{-1}$ (Stage 4) due to the narrowing discharge area (Figure 32 b, c, d).
Figure 32 – Changes in the groundwater flow and temperature fields caused by uplift and decreased cover thickness along the western part of the system. Red numbers represent maximum temperature; blue numbers represent temperatures at a distance of 10 km and 2 km deep, while orange numbers represent temperatures at 20 km and 1 km deep after a simulation time of 220 kyr. R1 and R2 show locations of recharge areas, D1 and D2 show locations of discharge areas. Vertical Darcy flux at the boundary between the two sub-systems is indicated by $q_z$. SP represents the location of the stagnation point.

5. Results of the heat transport simulation revealed, that the temperature field was primarily influenced by free-convection in the early evolutionary stages, with a maximum attained temperature of 84.3°C after a simulation time of 220 kyr. It was performed, that the temperature profile is increasingly influenced by cold meteoric water infiltration into the system, which led to the gradual decrease in maximum temperature of 98.6 °C in Stage 2 to 79.8 °C in Stage 4 (Figure 32 b, c). This tendency is in agreement with the findings of Kele et al. (2011), who revealed that travertines of the Buda Hills at the margin of the uplifted blocks
precipitated from warmer water (with temperatures between 20 and 65 °C) compared to modern water temperatures (between 20 and 28 °C).

6. As it was revealed by the numerical investigations, the simulated variation in temperature with depth is in accordance with the geothermal gradient only in the low-conductivity cover formation, as well as at the bottom of the carbonate (below approx. –3500 m depth, where the hydraulic conductivity is lower due to the assumed K-depth function). Within the carbonate unit, the vertical temperature gradient significantly deviates from the 40 °Ckm⁻¹ geothermal gradient. The larger the degree of convection, the more significant is the deviation from the geothermal gradient and from the pure conduction case, in agreement with the findings of An et al. (2015).

7. It was performed, that groundwater flow direction within the eastern cover formations significantly changed during system evolution from upward flow to partly downward flow (Figure 32). As showed by Mádl-Szőnyi et al. (2018), in the BTK pilot area, chloride-rich water (from antecedent seawater) was flushed from the pore space of the siliciclastic cover, thus increasing basinal fluid contribution to the BTK system. Results of the current study highlighted, in addition, that direct basinal fluid contribution was restricted in earlier stages of evolution (by stagnation point SP, see Figure 9 and Figure 10), and initiated only in the last stage of the system (ca. from Quaternary to recent time), contributing to the development of enhanced porosity.

Effects of low-permeability confining layers on groundwater flow and temperature distribution within the underlying permeable carbonate system

8. Based on the results of the simulations, uplift and consequent partial erosion of the cover layer controls the main character of the flow system which evolves from buoyancy-driven groundwater flow (Stage 1, 2 and 3) to dominantly gravity-driven flow (Stage 4). This is particularly evident along western part of the system, where flow intensity has significantly increased due to the increased meteoric infiltration through the uncovered carbonates in the recent state of the system (Stage 4). In contrary, the effect of gravity is completely attenuated within the carbonate by the presence of an uppermost low-permeability layer along the eastern sub-system, beneath which fluid flow is clearly driven by thermal free convection, in agreement with the results of numerical experiments of Yang et al. (2010).

9. It was revealed, that the period of cyclic temperature oscillations decreased from approx. 35 kyr period (in Stage 1) to approx. 15 kyr (in Stage 4) due to the reduced thickness of the left cover and the more efficient meteoric water infiltration. These changes led to an increase
of flow velocities (ex. $V_{z_{\text{max}}}$) increased from $10^{-7}$ ms$^{-1}$ in Stage 1 to $8 \times 10^{-7}$ ms$^{-1}$ in Stage 4) during system evolution and to the development of a more dynamic flow system.

**Relative importance of gravity and buoyancy as driving forces over geological time scales**

10. The importance of topography-driven flow in determining groundwater movement gradually increases in parallel with the increase of topographic gradient, as highlighted by the results of the numerical simulations. Topography-driven flow is more apparent within the cover layer, where flow gradually shifts toward the main discharge zone of the system. Within the carbonate, effects of groundwater forcing by gravity manifests in gradually reducing the number of upwellings from 6-8 (in Stage 1) to 3-4 (in Stage 4). However, buoyancy remains dominant until the complete erosion of low-permeability cover layer at the west ridge.

11. It was performed, that after the complete erosion of the cover from the western sub-system during Stage 4, gravity-driven flow completely overwrites the weaker buoyancy-driven flow. Within the uncovered sub-system of this stage, the evolved hydraulic gradient along the water table is more important than buoyancy in controlling the fluid flow system, and upwelling is forced by the regional hydraulic gradient toward the confined part of the system, where convection cells are maintained.

**Main influencing factors on flow field and temperature distribution**

12. As the results of the sensitivity analysis highlighted, the magnitude and depth-decay of hydraulic conductivity within the carbonate unit have the most significant effects on flow dynamics and temperature. In the initial state of the system (Stage 1), an order of magnitude decrease of hydraulic conductivity led to an increase of maximum temperature at the bottom of the carbonate by +42%, while in the partly unconfined current state of the system (Stage 4), $T_{(\text{max})}$ increased by +71%. The significant differences between $T_{(\text{max})}$ in these two stages can be attributed to the relative velocities within the partly unconfined system compared to the fully confined system, which result from the gradual change of meteoric water recharge during system evolution. However, induced changes in fluid dynamics caused minor modification in the overall flow and temperature field along the studied section.

The semi-synthetic numerical simulations of fluid flow and heat transport highlight the effects of paleo-recharge and confining formations, as well as the role of an evolving hydrodynamic system on heat distribution and dissipation. Effects of transient flow evolution on permeability, as well as on groundwater geochemistry in carbonate basins can be interpreted in further studies based on the results presented here, which can provide a suitable background to clarify more detailed site-specific mass and heat transfer related questions, such as i) How could groundwater flow affect
the properties of the carbonate range through long time scales and how will these properties provide feedback to the groundwater flow processes?; ii) How could large-scale changes in flow affect the residence time of groundwater in the different parts of the system?; and iii) How long does it take to leach brine water from the pores of the low permeable siliciclastic cover?

Moreover, in agreement with the study of Pollyea et al. (2015), the scale over which these processes operate is also important to determine since carbonate dissolution processes can best be interpreted based on the knowledge of physical processes operating at the relevant scale. Therefore, it is recommended to first place local scale studies into a larger scale groundwater flow context using regional investigations in order to determine general flow characteristics.
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a doktori értekezés szerzőjének aláírása

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