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

Theses of PhD dissertation

Timea Havril

Supervisor: Dr. Judit Mádl-Szőnyi
Eötvös Loránd University
Department of Physical and Applied Geology

Co-supervisor: Dr. John W. Molson
Université Laval
Department of Geology and Geological Engineering

Eötvös Loránd University, Doctoral School of Earth Sciences
Head of the doctoral school: Prof. Dr. Judit Bartholy

Doctoral Program of Geology and Geophysics
Head of the doctoral program: Prof. Dr. Szabolcs Harangi

Department of Physical and Applied Geology
Faculty of Science, Eötvös Loránd University

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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). Groundwater flow systems are 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.

In the case of deep carbonate systems (>3000 m deep), 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 evolution 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 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 BTK as an analogue system.

The main goal of the study was 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?

APPROACH: SNAPSHOT MODELS OF THE MAIN GEOLOGICAL EVOLUTIONARY STAGES

The numerical investigations of groundwater flow over geological time scales were placed into realistic geological evolutionary contexts through an example of the BTK pilot area. Four scenarios were tested to represent characteristic snapshots of the fluid evolution of the studied system and to examine the effects of tectonic uplift and erosion of confining siliciclastic strata above the carbonates.

1. In **Stage 1** (Early Late Miocene, approx. 10 Myr), a fully confined carbonate system was numerically interpreted. A uniform, 800 m thick low-permeability sedimentary cover was assumed to overlie the 3200 m thick permeable carbonate unit. 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.
2. During **Stage 2** (Early Pliocene, 5.3 – 3.6 Myr), vertical uplift of the western block began, thickness of the cover formation along the western subsystem was halved by erosion and in parallel, recharge of the system began by meteoric water infiltration. Due to the slightly elevated water table beyond the uplifting western part, open lateral boundaries can be assumed (inflow from the west, outflow toward east).

3. In **Stage 3** (Late Pliocene, 3.6 – 2.58 Myr) uplift of the eastern subsystem was also initiated (from approx. 4 Myr), which lead to the differentiated increase of topographic elevations and development of system boundaries. Additionally, an erosion base (and a water table minimum as well) evolved between the uplifting blocks (coinciding with what would eventually become the Danube basin in the case of the pilot area).
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 **Stage 4**. The eastern sub-basin remains confined. This stage reflects the most recent site characteristics.

An equivalent porous medium approach was applied (Abusaada and Sauter, 2013). Simplified, semi-synthetic snapshot models were simulated in a 2D vertical plane (in a 25 km wide, 4 km deep domain) using the Heatflow-Smoker finite element model (Molson and Frind, 2017) which couples density-dependent groundwater flow and heat transport. Sensitivity of the applied input parameters was examined within realistic uncertainty bounds for the initial (Stage 1) and recent (Stage 4) scenarios.

CONCLUSIONS AND THESES

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 gradually dissipate with time while new ones are born, eventually reaching a quasi steady-state pattern with temporally repeating similar patterns (Figure 1a). This vigorous, dynamic system is maintained due to the heat insulating role of the low-conductivity siliciclastic confining formation, in which a maximum temperature of

84.3 °C at the bottom of the carbonate unit is reached after a simulation time of 220 kyr.

2. As it was 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 1 b & c) 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 ($V_{z(max)}$ increased from 1.9×10^{-7} ms^{-1} in Stage 1 to 5.2×10^{-7} ms^{-1} in Stage 3; $V_{x(max)}$ increased from 7.3×10^{-8} ms^{-1} in Stage 1 to 2.3×10^{-7} ms^{-1} in Stage 3). The temperature profile is increasingly influenced by cold meteoric water infiltration into the system, which led to the gradual decrease in $T_{(max)}$ of 98.6 °C in Stage 2 to 88.8 °C in Stage 3.

3. It was demonstrated by the simulations, that cooling of the system significantly progressed to Stage 4 (Figure 1d). 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, in spite of the relatively high basal heat flux (100 mWm^{-2}) below the area. However, a heat accumulation developed within the eastern, covered carbonate sub-system. $T_{(max)}$ decreased by 18.8 °C (from 98.6 °C in Stage 2 to 79.8 °C in Stage 4) at the bottom of the system. 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 (T between 20-65 °C) compared to modern water temperatures (between 20-28 °C).

4. As the results of the simulations showed, discharge patterns changed significantly during the system evolution. Extension of the groundwater discharge area, developed as tectonic uplift initiated, gradually decreased from 17 km (Stage 2) to 15 km (Stage 3) and 13 km (Stage 4), respectively. Development of R2 recharge area during Stage 3 led to the compartmentalization of the discharge area (to D1, D2 and D3, see Figure 1c).

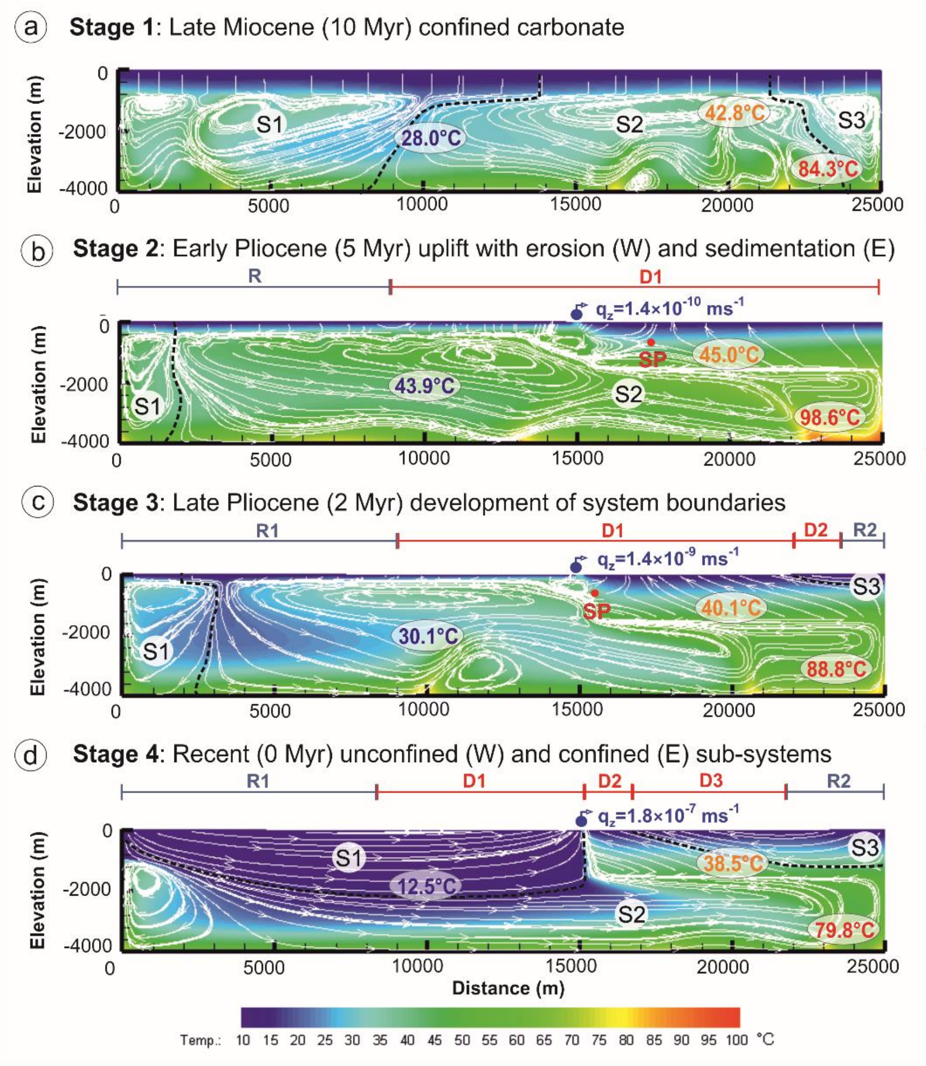

Figure 1 – Changes in the groundwater flow and temperature fields caused by uplift and decreased cover thickness along the western (W) part of the system. Red numbers represent maximum temperature; blue numbers represent temperatures at a distance of 10 km and 2 km deep, while orange numbers represent temperatures at 20 km and 1 km deep after a simulation time of 220 kyr. R1 and R2 show locations of recharge areas, D1, D2 and D3 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. It was revealed, that elimination of the stagnation point SP (see Figure 1 b&c) with time led to the direct discharge of regional flow at the boundary of the confined and unconfined sub-systems in the recent stage of the system (Stage 4). Darcy flux of discharging groundwater significantly increases with time by approx. 3 orders of magnitude (from 1.4×10^{-10} ms^{-1} in Stage 2 to 1.8×10^{-7} ms^{-1} in Stage 4) due to the narrowing discharge area (Figure 1 b, c & d).
6. As the results of the simulations showed, the 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 major part of 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.
7. It was shown, that groundwater flow direction within the eastern cover formations significantly changed during system evolution from upward flow to partly downward flow. 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 to the BTK system was restricted in earlier stages of evolution (by stagnation point SP, see Figure 1 b & c), 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. As the results of the simulation showed, presence of a low-permeability confining strata above the carbonate controls the main character of the flow systems (i.e. dominantly gravity-driven or buoyancy–driven) against the hydraulic gradient along the water table. 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 contrary, along the western part of the system, gravity-driven flow completely overwrites the weaker buoyancy-driven flow in parallel with the complete erosion of the cover.

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. $V_{z(max)}$ increased from 10^{-7} ms^{-1} in Stage 1 to 8×10^{-7} ms^{-1} in Stage 4) during system evolution, i.e. led to the development of a more dynamic flow system.

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

10. As highlighted by the results, differential tectonic uplift led to large-scale changes in the importance of different fluid driving forces (i.e. gravity and buoyancy) during system evolution. 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 of the system.

Main influencing factors on flow field and temperature distribution

11. As the results of the sensitivity analysis highlighted, the magnitude and depth-decay of hydraulic conductivity (K) of 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 K led to an increase of $T_{(max)}$ at the bottom of the carbonate by 42%, while in the partly unconfined current state of the system (Stage 4), $T_{(max)}$ increased by 71%. The significant differences between $T_{(max)}$ in these two stages can be attributed to the relative velocities, 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 field along the studied section.

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 results of the semi-synthetic paleo-hydrogeological simulations 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 heat distribution, permeability, as well as groundwater geochemistry in such 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.

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