

Supplementary material to

Topothermohaline convection – from synthetic simulations to reveal processes in a thick geothermal system

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1 Water density and molecular diffusion

In the synthetic and real case simulations, water density depended on the temperature, pressure and salt concentration as a sixth-order polynomial, a second-order polynomial and a linear function, respectively, following the formula of

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$$\rho_w(T, p, c) = \sum_{j=0}^6 \sum_{i=0}^2 a_{ij} p^i T^j + a_{00} \beta c, \quad (1)$$

where the first term provides the temperature- and pressure-dependent water density with an accuracy of 0.5% for a range of $p_{sat} < p \leq 100$ MPa and $0 \leq T \leq 350$ °C (Magri, 2009), and the second term is the linear effect of concentration on water density (Kohfahl et al., 2015). Coefficients for a_{ij} are reported in Magri (2009), while $\beta = 7.1 \cdot 10^{-4} \text{ l g}^{-1}$ was used after Kohfahl et al. (2015).

20 A quadratic form of Arrhenius law was applied to calculate the temperature-dependent molecular diffusion coefficient,

$$D_{diff}(T) = D_0 \exp \left[\frac{A}{T^2} + \frac{B}{T} + C \right], \quad (2)$$

where $D_0 = 10^{-9} \text{ m}^2 \text{ s}^{-1}$, temperature is given in K, constants of $A = -352\,450.2 \text{ K}^2$, $B = 163.6348 \text{ K}$ and $C = 4.247125$ were determined by fitting on data of Easteal et al. (1989) with an error of less than 0.02%.

25 2 Effect of mechanical dispersion in synthetic models

Mechanical dispersivity in synthetic models was neglected ($\alpha_L = \alpha_T = 0$) to focus on the dynamic interaction between topography-driven forced and free thermohaline convection. Here, an additional model is presented, in which $\alpha_L = 100 \text{ m}$ and $\alpha_T = 10 \text{ m}$ were applied in the base model ($H = 50 \text{ m}$, $q_{Tb} = 90 \text{ mW m}^{-2}$, $c_b = 70 \text{ g l}^{-1}$) to capture the effect of dispersion. Quasi-stationary solution

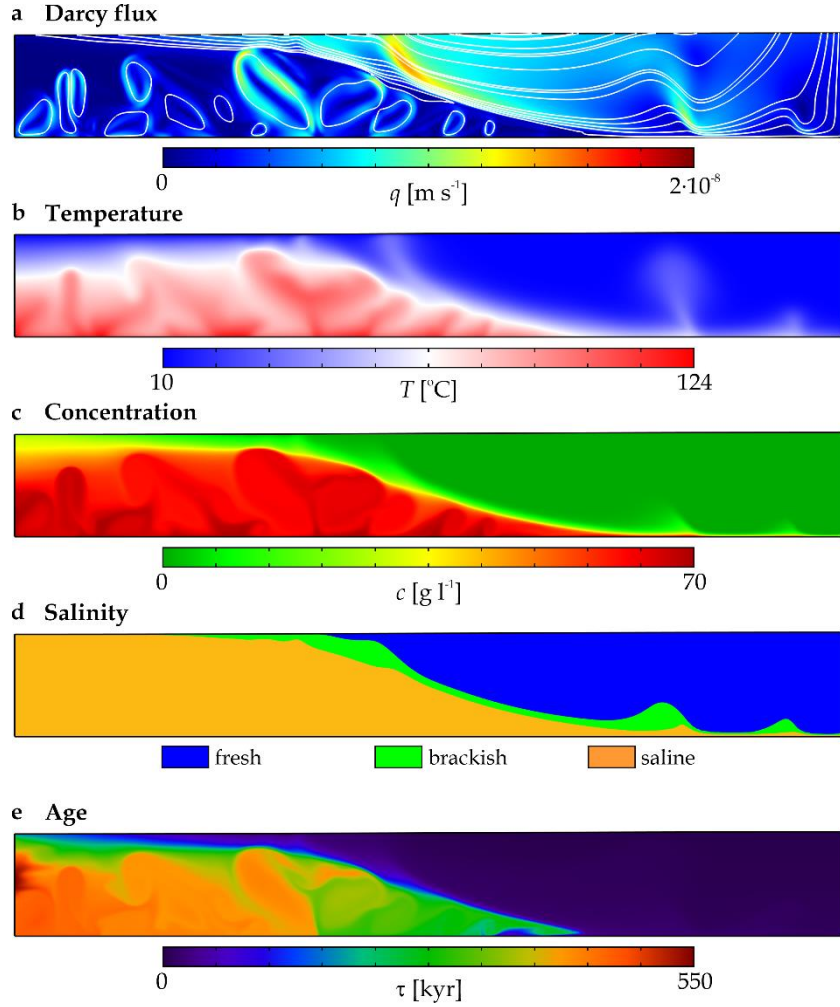


Figure S1 Snapshots of the (a) Darcy flux, (b) temperature, (c) salt concentration, (d) salinity zones and (e) groundwater mean age at $t=3$ Myr after the initial state in the base model (Table 2) including longitudinal ($\alpha_L=100$ m) and transverse ($\alpha_T=10$ m) dispersivity. (a) Streamlines illustrate the flow direction. (d) Salinity zones: freshwater (blue), brackish water (green) and saline water (orange).

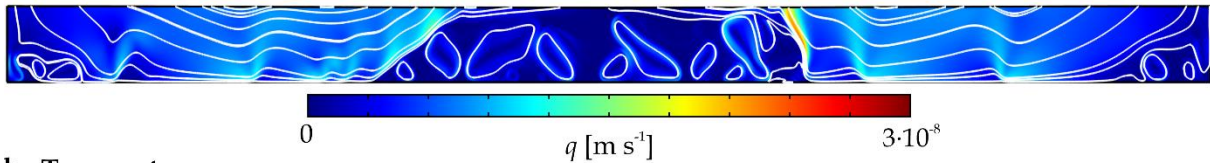
after 3 Myr is presented in Figure S1 showing that a more extensive thermohaline dome developed beneath the discharge zone (left) compared to the base model (Fig. 2) due to the facts that (1) the transverse dispersion increased concentration flux through the bottom boundary, and (2) the longitudinal dispersion effectively mixed the groundwaters in the basin. The phenomenon is very similar to the behaviour of the saltwater zones in synthetic topohaline convection models, where the effect of dispersivity was investigated in detail (Galsa et al., 2022). The relative area of the saline water zone increased from $A_{sal}=35\%$ to 50% resulting in higher average concentration (from $c_{av}=12.2$ g l⁻¹ to 27.1 g l⁻¹), temperature (from $T_{av}=34.7$ °C to 45.8 °C) and water age (from $\tau_{av}=121$ kyr to 170 kyr) as well as lower Darcy flux (from $q_{av}=4.79 \cdot 10^{-9}$ m s⁻¹ to 4.20 m s⁻¹). Thus, mechanical

dispersion, like other physical/numerical parameters (e.g. temperature- and pressure-dependent viscosity, boundary conditions), strongly influences the behaviour of the complex system.

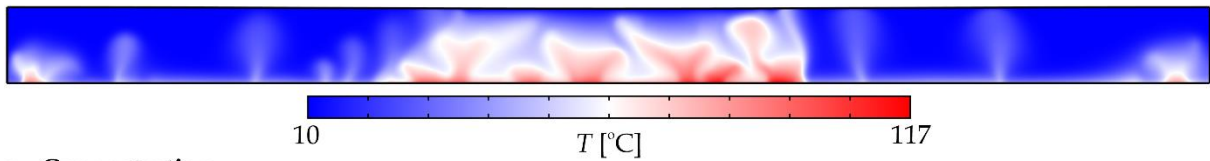
3 Effect of the side wall on the thermohaline dome

Undoubtedly, all boundary conditions affect the numerical solution obtained in the model domain, whether it is a synthetic or real model, whether it refers to flow, temperature, salt concentration or water age. If a thermohaline dome is formed in a synthetic model, it always develops beneath the discharge zone, near the vertical no-flow (Darcy flux), thermally insulating (temperature) and no-flux (salt concentration and water age) boundary. Therefore, the qualitative and quantitative impact of the lateral boundary on the topotharmohaline system evolving in the synthetic model was investigated, and in particular on the

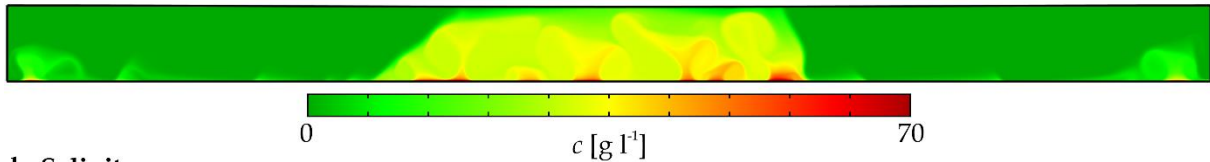
a Darcy flux



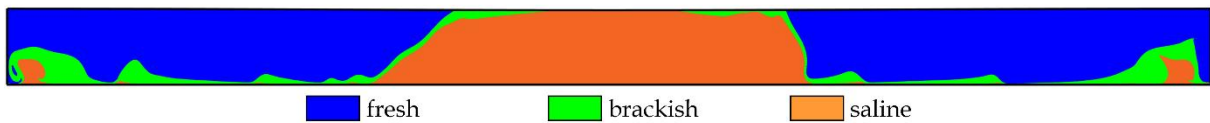
b Temperature



c Concentration



d Salinity



e Age

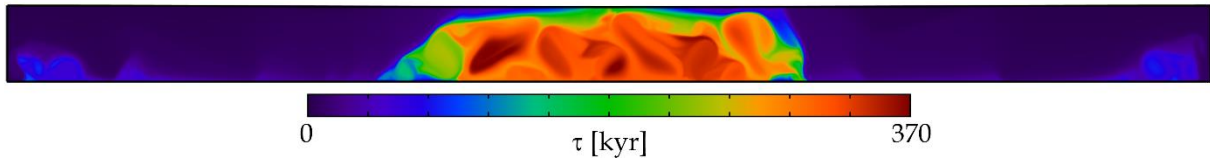


Figure S2 Snapshots of the (a) Darcy flux, (b) temperature, (c) salt concentration, (d) salinity zones and (e) water age at $t=3.5$ Myr after the initial state in the base model (Table 2) with doubled model domain. (a) Streamlines illustrate the flow direction. (d) Salinity zones: freshwater (blue), brackish water (green) and saline water (orange).

thermohaline dome. In order to eliminate the side boundary effect, two sinusoidal unit basins were merged with the parameters
45 of the base model (Table 2), in which the discharge zone was located in the middle of the domain and thus unaffected by the
side boundaries and boundary conditions.

The thermohaline dome also formed under these conditions (unaffected by lateral boundaries), so it is clear that the
dome beneath the discharge zone is the hydro-geophysical consequence of the system, and not an artificial phenomenon caused
by the vertical boundary condition (Fig. S2). The thermohaline dome developed in the doubled model domain is now
50 dynamically bounded on both sides, and intense thermohaline convection occurs within it. Comparing its quantitative
characteristics with the base model, it was found that the relative size of the thermohaline dome decreased from $A_{sal}=35\%$ to
31%, and its average Darcy flux was essentially unchanged (from $q_{sal}=2.64\cdot 10^{-9} \text{ m s}^{-1}$ to $2.76\cdot 10^{-9} \text{ m s}^{-1}$), its temperature, salt
concentration and age decreased from $T_{sal}=62.9\text{ }^{\circ}\text{C}$, $c_{sal}=33.4 \text{ g l}^{-1}$ and $\tau_{sal}=322 \text{ kyr}$ to $59.2\text{ }^{\circ}\text{C}$, 29.3 g l^{-1} and 255 kyr ,
respectively. Overall, it can be concluded that the thermohaline dome continues to form beneath the discharge zone, slightly
55 weakened in its quantitative character, but the features of topothermohaline convection are consistent with the phenomena in
the unit basin presented in the paper.

4 Effect of non-constant viscosity and bottom boundary condition in the BTK model

For simplicity and to save computational resources, the numerical calculations were performed at constant water viscosity.
The present simulation illustrates the effect of temperature-, pressure- and concentration-dependent viscosity along the BTK
60 section. The value of dynamic viscosity in the present hydrogeological model varied between $\mu=10^{-4}$ and $1.3\cdot 10^{-3} \text{ Pa s}$ and was
mainly influenced by the temperature. In addition, an impermeable layer ($k=0 \text{ m}^2$) of 1 km thickness was placed below the
model domain, and the lower boundary conditions — which were the same as those described in Section 3.2.1 — were imposed
at the bottom of this layer.

These two factors resulted in a more efficient reduction of salinity in the deep, confined reservoir because (1) the
65 reduced viscosity due to high temperature led to more intense thermohaline convection and (2) salt was only transported by
diffusion through the lower impermeable layer (Fig. S3). The lower salinity and reduced viscosity intensified the flow, thus
slightly decreasing the water age. While no change in the maximum reservoir temperature was observed, its size was slightly
decreased based on the model calculation. In contrast, in the regions near the discharge zone and below the Oligocene cover
(HS6), a warming of a few degrees was observed, which is most likely a consequence of the more intense upwelling caused
70 by the reduced viscosity. However, in terms of the basic characteristics of the BTK system, no substantial changes were found
due to the two modified parameters (variable viscosity and modified lower boundary condition), topography-driven
groundwater flow in the unconfined karst area and thermohaline convection in the confined reservoir being the dominant
groundwater flow regimes. A reservoir with high geothermal potential has formed beneath the clayey cover containing
saline/brackish and aged water, which can persist over geological time scales. We mention that BTK models were also
75 calculated in which only one factor was changed (variable viscosity or bottom impermeable layer). Their solutions fell between

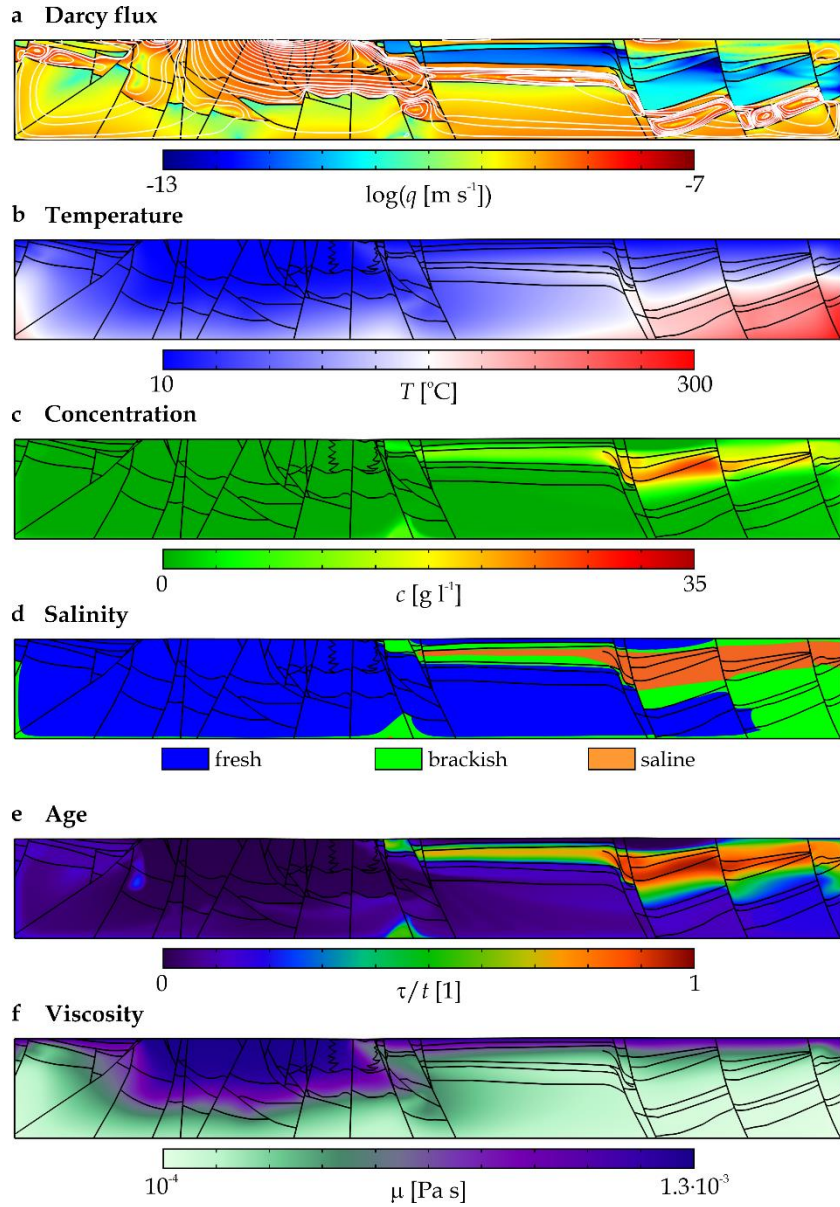


Figure S3 Solution of the topothermohaline convection in the Buda Thermal Karst system applying temperature-, pressure and concentration-dependent viscosity and a lower impermeable layer (not shown). Distributions of (a) the Darcy flux, (b) the temperature, (c) the salt concentration, (d) the salinity zones, (e) the water age and (f) the dynamic viscosity at 1 Myr. The direction of Darcy flux is illustrated with streamlines (white). The groundwater mean age, τ is normalized by the simulation time, t .

the two models presented (Fig. 10 and Fig. S3) in terms of salt concentration. The presence of the bottom impermeable layer increased the water age in the confined reservoir, while the temperature-dependent viscosity slightly decreased the temperature.

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