

**Elucidating the relationship between aquifer heterogeneity and thermal dispersivity
using stochastic heat transport simulations**

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Rescaling between mass and heat transport equations

It is often mentioned that the mass transport equation and the heat transport equation are mathematically equivalent (e.g. Shook 2001, Hecht-Méndez et al. 2010, Rau et al. 2010 etc). Although it is a fact, it can easily lead to some misunderstandings. Common conclusion from mathematical equivalence is that heat and mass transport give similar results, and the difference between the two solutions can be corrected by using the retardation factor. However, it is only true under appropriate conditions.

First of all, typical geothermal and typical mass transport problems have different boundary conditions. In a typical deep geothermal problem, where cold water is injected into a permeable porous medium, the conductive heat flux affects the temperature of the injected cold water across the horizontal boundaries of the aquifer, leading to a quasi-parabolic shape of the thermal front. In contrast, no-flux boundary conditions are applied in a typical mass transport problem due to the low mechanical diffusion (thermal diffusion is several orders of magnitude greater than mechanical diffusion). Different boundary conditions have crucial effects on the results, which is why the retardation factor alone is not sufficient to rescale the results. The retardation factor can only be used if the conduction is negligible (in case of large Péclet number).

In order to illustrate the differences, we have accomplished some simple simulations to investigate the propagation of the concentration front and the thermal front in a homogeneous medium in the absence and in the presence of thermal conduction. Figure S1. shows the solute front (Fig. S1.a) and thermal front in the absence (Fig S1.b) and in the presence (Fig S1.c) of thermal conduction at 30 years of the simulation after the injection. The solute fronts and the thermal front without thermal conduction are regular vertical lines, and indeed, the thermal front can be calculated from the concentration front by applying the retardation factor. However, if the thermal conduction is present, the shape of the thermal front is more complex, since the vertical heat flux from hot bedding aquitards gradually heats the injected water (Fig. S1.c). This behavior does not correspond to an effective retardation factor and thus is cannot be rescaled from the solute front. Note, the difference is even greater as time goes on and thermal conduction has more time to warm up the pore water (e.g. in longer model domain or at lower Darcy flux). As a consequence, the mass transport and heat transport cannot be rescaled due to the different boundary conditions.

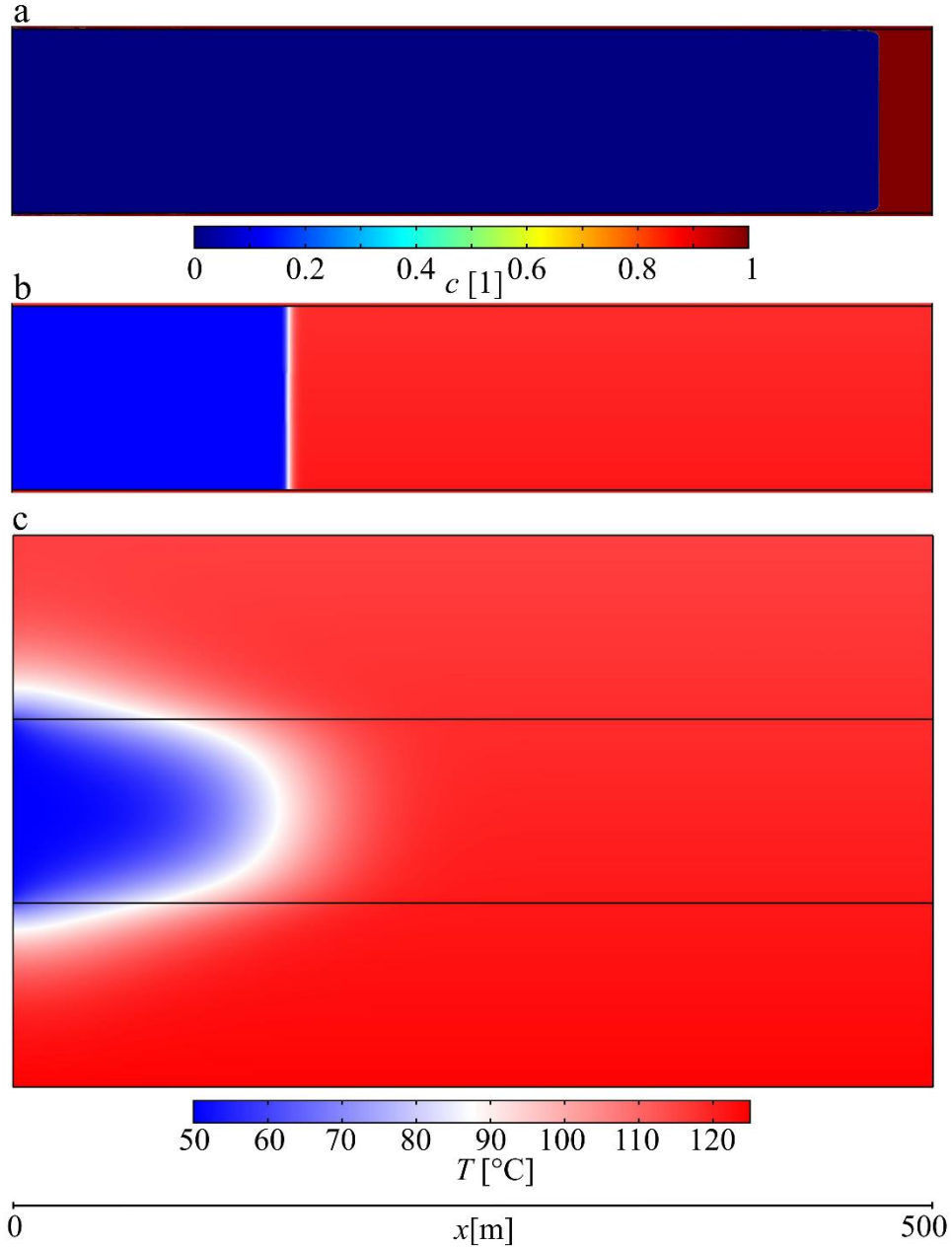


Fig. S1 (a) Solute front and thermal front (b) in the absence and (c) in the presence of thermal conduction at 30 yr after water injection into homogeneous aquifer ($L=500$ m, $q_{in}=10^{-7}$ m/s).

This is confirmed by Figure S2, where the time series of the outlet temperature show quantitatively the discrepancy. The solute front travels $L=500$ m in 31.8 years in the numerical model with homogeneous media at $q_{in}=10^{-7}$ m/s, $\Phi=0.2$. While the thermal front needs 99.7 yr to travel 500 m with the same parameters in the absence of thermal conduction. This time (99.7 yr) can be calculated by the retardation factor (Hecht-Méndez et al. 2010, Molina-Giraldo et al. 2011, Rau et al. 2012) using the model parameters from the paper:

Solute front velocity:

$$v_s = \frac{q_{in}}{\Phi} = \frac{10^{-7} \text{ m/s}}{0.2} = 5 \cdot 10^{-7} \text{ m/s} \quad (1)$$

$$t_s = 31.7 \text{ yr} \quad (2)$$

Thermal front velocity:

$$v_t = \frac{1}{R_t} \cdot q_{in} = \frac{\rho_w \cdot c_w}{\rho_m \cdot c_m} \cdot q_{in} = \frac{\rho_w \cdot c_w}{\phi \cdot \rho_w \cdot c_w + (1-\phi) \cdot \rho_m \cdot c_m} \cdot q_{in} =$$

$$= \frac{1000 \frac{\text{kg}}{\text{m}^3} \cdot 4200 \frac{\text{J}}{\text{kg K}}}{0.2 \cdot 1000 \frac{\text{kg}}{\text{m}^3} \cdot 4200 \frac{\text{J}}{\text{kg K}} + 0.8 \cdot 2500 \frac{\text{kg}}{\text{m}^3} \cdot 900 \frac{\text{J}}{\text{kg K}}} \cdot 10^{-7} \frac{\text{m}}{\text{s}} = 1.59 \cdot 10^{-7} \frac{\text{m}}{\text{s}} \quad (3)$$

$$t_t = 99.7 \text{ yr} \quad (4)$$

Overall, the rescaling between results from solute transport and heat transport cannot be done in the presence of thermal conduction owing to the different boundary conditions used in the numerical models, although the solute and heat transport equations are mathematically equivalent.

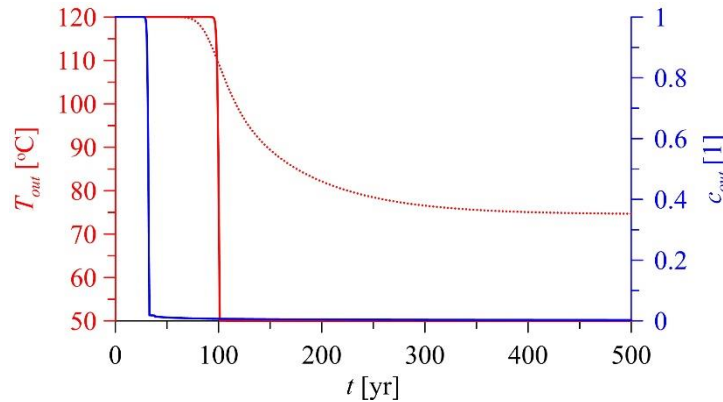


Fig. S2 Outlet solute (blue) and temperature time series at $x=500$ m in the absence (red continuous line) and in the presence of thermal conduction (red dotted line).

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