The impact of aquifer heterogeneity on the performance of aquifer thermal energy storage

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[1] Heterogeneity in hydraulic properties of the subsurface is not accounted for in current design calculations of aquifer thermal energy storage (ATES). However, the subsurface is heterogeneous and thus affects the heat distribution around ATES wells. In this paper, the influence of heterogeneity on the performance of a doublet well system is quantified using stochastic heat transport modeling. The results show that on average, thermal recovery decreases with increasing heterogeneity, expressed as the lognormal standard deviation of the hydraulic conductivity field around the doublet. Furthermore, heterogeneity at the scale of a doublet ATES system introduces an uncertainty in the amount of expected thermal interference between the warm and cold storage. This results in an uncertainty in thermal recovery that also increases with heterogeneity and decreases with increasing distance between ATES wells. The uncertainty in thermal balance due to heterogeneity can reach values near 50 percent points in case of regional groundwater flow in excess of 200 m/yr. To account for heterogeneity whilst using homogeneous models, an attempt was made to express the effect of heterogeneity by an apparent macrodispersivity. As expected, apparent macrodispersivity increases with increasing heterogeneity. However, it also depends on well-to-well distance and regional groundwater velocity. Again, the uncertainty in thermal recovery is reflected in a range in the apparent macrodispersivity values. Considering the increasing density of ATES systems, we conclude that thermal interference limits the number of ATES systems that can be implemented in a specific area, and the uncertainty in the hydraulic conductivity field related to heterogeneity should be accounted for when optimizing well-to-well distances.

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1. Introduction

[2] Due to increasing energy demand and concern about emission of greenhouse gasses, groundwater-based heating and cooling systems are receiving attention worldwide. Among the different types of energy storage systems, aquifer thermal energy storage (ATES) is suitable for largescale applications like residential areas, shopping malls, and utility buildings. Aquifer thermal energy storage is a technology in which sensible heat is temporarily stored in the subsurface through injection and withdrawal of groundwater [Dickinson et al., 2009; Kim et al., 2010]. The heat capacity of the groundwater is used to transfer heat between a building and the aquifer. Application of ATES

results in savings on conventional resources used for heating or cooling, and leads therefore to a reduction of (1)dependence on these resources, (2) costs, and (3) CO₂ emissions.

[3] ATES systems in regions with a cold-warm periodicity, like Netherlands, commonly operate in a seasonal mode [Dickinson et al., 2009; Koenders, 2007]. In summertime, cool groundwater is extracted and used to cool down a building. The heated groundwater is injected back into the aquifer through a different well creating a storage of heated groundwater (i.e., warm wells). In wintertime, the flow direction in the system is reversed: the heated groundwater is extracted, used to heat the building and create a cold storage (i.e., cold wells).

[4] The storage efficiency of each ATES well is expressed as thermal recovery (TR), defined as the ratio between thermal energy that is extracted from the subsurface and what was stored (equation (1)).

$$TR = \frac{\int_{\text{extraction}} c_{water} \cdot Q \cdot (T - T_{natural}) \cdot dt}{\int_{\text{injection}} c_{water} \cdot Q \cdot (T - T_{natural}) \cdot dt}$$
(1)

[5] Here, c_{water} is the volumetric heat capacity of water, Qis the pumping rate, T is the temperature of the water that is

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injected or extracted, $T_{natural}$ is the natural temperature of the aquifer, and dt is a time increment. The integrals in equation (1) can be evaluated over any time period. In our analysis, we will consider each cycle of storage and subsequent recovery separately.

[6] Modeling studies of a single ATES well show that thermal recovery is always lower than 100% as a result of heat loss by regional groundwater flow [Kangas and Lund, 1994] and heat conduction [Chevalier and Banton, 1999; Doughty et al., 1982; Sauty et al., 1982a]. When the wells for storing cold and warm water are built close together, thermal recovery may be further reduced by thermal interference between the wells [Kim et al., 2010; Kowalczyk and Havinga, 1991; Lee, 2010; Lee and Jeong, 2008]. On the other hand, thermal recovery of wells in multiwell systems may increase due to thermal interference between wells with similar storage temperature [Bakr et al., 2013].

[7] Reports of thermal recoveries for actual systems are scarce. Sauty et al. [1982b] report thermal recoveries between 18.9% and 68% for several small-scale field experiments. The lower value for thermal recovery was attributed to the fact that energy was stored close to the surface, leading to high heat loss to the surface. For a larger field experiment, where 55.000 m³ water of 55°C was injected and recovered during a 6 month cycle, Molz et al. [1981] report thermal recovery values of 66% and 76% for two successive storage and recovery cycles. For two similar field experiments, where water of 58.5 and 81°C was injected, recoveries of 56% and 45% were achieved [Molz et al., 1983]. The lower value is explained by increased buoyancy flow due to higher storage temperature. More recently, Sommer et al. [2013] reported a 7 year average thermal recovery of 82% for cold storage and 68% for heat storage for an operational ATES site in Netherlands.

[8] Since its introduction in the 1970s, use of ATES has experienced large growth worldwide. Due to increasing demand for sustainable energy, this trend is expected to continue [Dickinson et al., 2009]. In Netherlands, ATES is already used as a standard technique for utility buildings such as offices, hospitals, and public buildings [Stolker, 2009]. Due to limited space in urban areas. thermal interference between wells is a major concern for large-scale application of ATES. An example of an ATES system, where extraction temperatures are negatively influenced by thermal interference in the subsurface is given by Ferguson and Woodbury [2006]. To avoid thermal interference guidelines exist on well-towell distance [Haehnlein et al., 2010; NVOE, 2006]. For ATES systems, it is convenient to express well-to-well distance in terms of thermal radii. The thermal radius (R_{th}) is defined as the maximum distance of the thermal front from the injection well in a homogeneous medium and neglecting vertical flow, advection by regional flow, thermal conduction and dispersion (equation (2)).

$$R_{th} = \sqrt{\frac{c_{water} \cdot V}{c_{aquifer} \cdot \pi \cdot H}}$$
(2)

[9] Here, $c_{aquifer}$ is the volumetric heat capacity of the aquifer (groundwater and aquifer matrix), V is the volume of water that is injected in one storage cycle, and H is the length of the well screen.

[10] Literature shows diversity in recommended well-towell distances. *Kim et al.* [2010] report on the basis of numerical modeling that the recovery of thermal energy is not significantly affected when the wells are separated by more than one thermal radius. *Kowalczyk and Havinga* [1991] report an optimal well-to-well distance between 1 and 2 thermal radii for heat storage and as far as possible for cold storage. The Dutch society for subsurface heat storage (NVOE) advises a well-to-well distance of at least three thermal radii to avoid thermal interference [*NVOE*, 2006].

[11] These guidelines and design calculations are based on the assumption of a homogeneous subsurface, while studies for unconsolidated aquifers report widely varying degrees of hydraulic heterogeneity, of up to 2.1 in terms of the log conductivity standard deviation (σ) [Dagan and Neuman, 1997; Gelhar, 1993; Hoeksema and Kitanidis, 1985; Rehfeldt et al., 1992; Sudicky, 1986; Vereecken et al., 2000]. Reported correlation lengths of aquifers are in the order of cm to km [Gelhar, 1993]. Especially heterogeneity in the horizontal direction at the scale of an ATES system or larger may create preferential pathways, reducing ATES performance due to increased advective heat loss or thermal interference between ATES wells.

[12] The role of hydraulic heterogeneity of the subsurface related to ATES performance has received little attention in the literature. Previous research includes the modeling of a single ATES well in a heterogeneous aquifer under stagnant flow conditions [Ferguson, 2007] and the influence of heterogeneity on thermal recovery of a group of ATES systems [Caljé, 2010]. Ferguson [2007] uses the geostatistical properties from the Borden aquifer [Woodbury and Sudicky, 1991] and a carbonate rock aquifer [Kennedy and Woodbury, 2002] to determine the influence of heterogeneity on the recoverability of thermal energy. For the Borden aquifer $(\sigma = 0.261)$, he calculated a reduction of 5.5% in energy recovered with respect to the homogeneous model while for the more heterogeneous carbonate rock aquifer ($\sigma = 1.6$) a reduction of 8.2% is reported. Temperature measurements around ATES wells [Allen and Bridger, 2003; Bridger and Allen, 2010; Sommer et al., 2013] indicate that heterogeneity gives rise to preferential pathways and short-circuiting between ATES wells. This may not only result in a different thermal efficiency than expected based on design calculations, but also in an increased spatial extent that is used by an individual ATES system, which is not available for other systems in the surrounding [Ferguson, 2007]. To avoid thermal interaction, wells in heterogeneous media should be placed farther apart than in homogeneous media, leading to a larger spatial claim in the subsurface.

[13] This research elaborates on the effect of heterogeneity on the storage performance of ATES. Heat transport modeling is applied to simulate operation of a doublet ATES system in a subsurface with 3-D heterogeneous hydraulic conductivity. Sensitivity analyses are conducted to assess the influence of heterogeneity under different design condition (well-to-well distance, orientation of the doublet with respect to regional groundwater flow) and hydrogeological conditions (groundwater velocity). Since the number of noninterfering ATES systems that can be realized in an area depends on well-to-well distance, this research supports assessment of the potential contribution of ATES to sustainability goals.



Figure 1. Example of a heterogeneous subsurface ($\mu = 3.2$, $\sigma = 1$, $\lambda_h = 104.1$ m, $\lambda_v = 2$ m). The colors indicate log conductivity in log(m/d).

2. Method

[14] To address the statistical uncertainty in groundwater flow and heat transport in heterogeneous media, a Monte Carlo approach was applied [*Freeze*, 1975]. Ensembles of synthetic 3-D heterogeneous hydraulic conductivity fields were generated, in which the operation of a doublet ATES system was simulated for a period of 10 years. The heterogeneous conductivity fields were generated using GSLIB [*Deutsch*, 1997]. Spatial correlation was defined as an exponential covariance function, described by a horizontal and vertical correlation length. The 3-D fields that were generated with GSLIB have a zero mean and unit standard deviation. These were converted to lognormal hydraulic conductivity fields using equation (3).

$$k = e^{\mu + \sigma \cdot r} \tag{3}$$

[15] Here, k is hydraulic conductivity and r is the spatially correlated random variate generated by GSLIB. The values μ and σ define the mean and standard deviation of the lognormal hydraulic conductivity field. An example is given in Figure 1. Preliminary tests showed that the median thermal recovery of an ensemble converges between 10 and 30 members. Therefore, it was decided to limit the ensemble size to 50 members. In addition to the ensemble median, the 10th and 90th percentiles were calculated to show the spread in the results. These percentiles were chosen as being more robust estimators than the minimum and maximum values. The method of *Helsel and Hirsch* [1992] was applied to check the precision at which the percentiles could be estimated.

[16] Modflow [*Harbaugh*, 2000] and MT3DMS [*Zheng and Wang*, 1999] were used to model water and heat transport. MT3DMS was originally designed to model solute transport. Due to similarity between the solute and energy transport equation MT3DMS can be applied to model heat transport by adopting the following transformations

[Hecht-Mendez et al., 2010; Thorne et al., 2006]. The thermal diffusion coefficient $(D_T) = k_{bulk} / (n \cdot \rho \cdot c_{p,water})$, where k_{bulk} is the bulk thermal conductivity of the aquifer, n is porosity, ρ is the density of water and $c_{p,water}$ is the specific heat capacity of water; the thermal distribution coefficient $(K_d) = c_{p,solid}/(c_{p,water} \cdot \rho)$, where $c_{p,solid}$ is the specific heat capacity of the solid phase. The dimensions of the ATES system have been chosen to represent ATES systems typically applied for utility buildings [Dickinson et al., 2009; Paksov et al., 2004; Zuurbier et al., 2013]. The horizontal grid size was set at 1/10 of the thermal radius (5.2 \times 5.2 m). The 3-D heterogeneous conductivity field generated through GSLIB describes the aquifer in which ATES is applied. The aquifer consists of 20 layers with a thickness of 1 m each. The aquifer is bounded on the top and bottom by aquitards. Both aquitards are discretized by eight layers with thicknesses increasing by a factor 1.5 starting from 1 m at the edge of the aquifer. Test calculations showed that further reducing the grid size or increasing the aquitard thicknesses does not influence the calculated thermal performance of the ATES system. The length of the well screens is equal to the thickness of the aquifer layers in the model. To simulate regional groundwater flow, a constant discharge boundary condition was applied to the south boundary and a constant head to the north boundary. The east and west have no-flow boundaries. The north boundary also has a constant temperature equal to the initial aquifer temperature of 10°C. In the reference model scenario, the doublet was oriented perpendicular to the regional groundwater flow (if present), so that both wells would be affected equally by advective heat loss (wells C1 and W2 in Figure 2). The wells were modeled using the multinode well (MNW) package [Halford et al., 2002; Zheng, 2010]. For wells that are screened over multiple layers, the MNW package distributes the total prescribed well flow rate over the different nodes according to the calculated pressure. Furthermore, a flux weighted extraction temperature in the well has been calculated.



Figure 2. Top view of model, with well locations for several scenarios and boundary conditions indicated. The colors indicate log conductivity (see Figure 1, for scale). All scenarios use only two wells (or one to simulate infinite well-to-well distance). The reference case combines C1 (cold well) and W2 (warm well). The distance between wells is varied by changing the location of the warm well to W1 or W3. The angle with regional flow is varied by selecting wells C2 and W4 (45°) or C3 and W5 (0°).

[17] The ATES system was modeled using fixed injection temperatures and a closed water volume balance, i.e., equal injection and extraction rates (Q). Injection temperatures were set at 14°C (summer) and 6°C (winter). The initial aquifer temperature was fixed at 10°C throughout the whole domain. The temperature differences due to thermal storage are small enough to neglect the temperature dependency of density and viscosity [*Bridger and Allen*, 2010; *Fossoul et al.*, 2011; *Zuurbier et al.*, 2013]. Each storage and recovery cycle consists of 4 months of constant operation of the ATES system during summer and winter, with a 2 month passive storage phase in between (Figure 3). This mimics the operational strategy commonly observed in actual systems [*Dickinson et al.*, 2009; *Zuurbier et al.*, 2013].

[18] The results were analyzed for thermal recovery (TR, equation (1)) and thermal balance (equation (4)), expressed in the energy balance ratio (EBR) [*Koenders*, 2007].



Figure 3. Yearly time evolution of pumping rate and temperature in the wells for a typical model run. Injection temperatures are indicated with a solid line. The pumping rate out of the cold well and into the warm well (summer operation) is defined positive, and the pumping rate out of the warm well and into the cold well (winter operation) is defined negative.

$$EBR = \frac{E_{cold}^{extracted} - E_{warm}^{extracted}}{E_{cold}^{extracted} + E_{warm}^{extracted}}$$
(4)

[19] The amount of cold energy that is extracted from the subsurface $(E_{cold}^{extracted})$ is given by:

$$E_{cold}^{extracted} = \int_{\text{cold extraction}} c_{water} \cdot Q \cdot abs \left(T_{extr} - T_{inj} \right) \cdot dt \qquad (5)$$

[20] Here, T_{extr} is the temperature of the water being extracted, T_{inj} is the temperature of the injected water and the integration is over the period of cold water extraction (cooling of the building). For the amount of warm energy extracted, the same equation was used, now integrating over the period of warm water extraction (heating).

[21] As mentioned before, the dimensions of the reference ATES system (Table 1) are representative of a typical ATES system in Netherlands. However, the effect of heterogeneity on the performance of the ATES system may depend not only on the degree of heterogeneity but also on the configuration of the ATES system and hydrological conditions. To explore the effect of these conditions on ATES performance, local sensitivity analyses were performed by varying the following parameters separately with respect to the reference case: (1) horizontal correlation length, (2) log conductivity standard deviation, (3) well-to-well distance, (4) regional groundwater flow velocity, and (5) orientation of the doublet system with respect to the regional flow (Table 2).

[22] Finally, the possibility of representing heterogeneity by an apparent macrodispersivity is investigated. This could enable the use of homogeneous models, which are less computationally demanding. To this end, for each heterogeneous scenario, a series of homogeneous models was generated with longitudinal dispersivity ranging from 0 to 50 m, where the reference value is a dispersivity of 0 m (Table 1). The hydraulic conductivity field for the homogeneous models is obtained by setting σ to zero in equation (3). Model results for each series were used to derive a relation between model dispersivity and calculated thermal recovery. Apparent values for macrodispersivity were determined by fitting the thermal recovery of the ATES system as calculated by the heterogeneous model with the thermal recoveries of the series of homogeneous models with varying dispersivity. The practical applicability of an apparent macrodispersivity to assess the uncertainty in thermal recovery associated with aquifer heterogeneity is discussed in some detail.

3. Results

[23] First, the effects of heterogeneity on the performance of a typical doublet ATES system are presented (the reference case, Table 1), followed by the results of the sensitivity analysis (Table 2) and the apparent dispersivity estimations.

3.1. Reference Case

[24] Figure 4 shows the thermal recovery for the first 10 storage and recovery cycles for the reference model. Plotted are the thermal recovery of an ATES system in a homogeneous subsurface and the median thermal recovery of the ensemble of heterogeneous models together with the 10

Table 1. Model Parameter Values for the Reference Case

Grid cells (rows \times columns \times layers)	140 imes 100 imes 36	
Cell size (m)	$5.2 \times 5.2 (0.1 \cdot R_{th})$	
Cell thickness layers 1–36 (m)	17.1; 11.4; 7.6; 5.1; 3.4; 2.3; 1.5; 1; 20 × 1; 1; 1.5; 2.3; 3.4; 5.1; 7.6; 11.4; 17.1	
Distance between wells (m)	$104.1 (2 \cdot R_{th})$	
Pumping rate (m ³ /storage cycle)	100,000	
Ensemble size	50	
Horizontal correlation length (m)	$104.1 (2 \cdot R_{th})$	
Vertical correlation length (m)	2	
Average horizontal hydraulic conductivity (log(m/d))	3.2	
Log conductivity standard deviation	1	
Vertical hydraulic conductivity (m/d)	Horizontal hydraulic conductivity/10	
Porosity (–)	0.3	
Regional flow velocity (m/yr)	0	
Dispersivity (m)	0	
Water density $(kg/m^3)^a$	999.7	
Water heat capacity $(J/kg/K)^{a}$	4192.1	
Water thermal conductivity $(W/m/K)^{a}$	0.58	
Solid density $(kg/m^3)^b$	2643	
Solid heat capacity (J/kg/K) ^b	652	
Solid thermal conductivity $(W/m/K)^{b}$	7.69	
Thermal distribution coefficient (m ³ /kg)	0.000156	
Thermal diffusion coefficient (m^2/d)	0.382	

^aWater and aquifer properties from *Lide* [1993].

^bWater and aquifer properties from *Thorne et al.* [2006].

and 90 percentiles. For both the homogeneous and heterogeneous case, thermal recovery increases with every storage and recovery cycle. This has also been observed in previous modeling studies [Doughty et al., 1982; Lee and Jeong, 2008; Sauty et al., 1982a] and in field experiments [Molz et al., 1981; Sommer et al., 2013]. During the first cycle, part of the thermal energy is lost due to thermal diffusion and dispersion. In the following cycles, the amount of lost energy gets smaller as the surroundings have already warmed up or cooled down because of energy dissipation in the previous cycles. Figure 4 shows that for the reference system, thermal recovery in a homogeneous aquifer reaches 75.7% in the 10th recovery cycle. The median thermal recovery in a heterogeneous aquifer is 5.8 pp (percent point) lower than in a homogeneous aquifer. Moreover, uncertainty in the exact conductivity field in case of a heterogeneous aquifer results in an uncertainty in thermal recovery between 67.7 and 72.9% indicated by the 10th and 90th percentiles. Precision of the percentiles is within 1 pp (Table 3).

 Table 2. Overview of Scenarios Considered for Sensitivity

 Analysis

Parameter (unit)	Range in Parameter Value	Reference Case
Horizontal correlation length (thermal radii)	0.2, 1, 2, 5, 20 (=10.4, 52.0, 104.1, 156.1, 1040.7 m)	2 (=104.1 m)
Standard deviation Well distance (thermal radii)	$\begin{array}{c} 0,0.5,1,2\\ 1,1.5,2,3,\infty^{a}\\ (=\!52.0,78.1,104.1,\\ 156.1,\infty\ m) \end{array}$	1 2 (=104.1 m)
Regional flow velocity (m/yr) Angle between regional flow ^b and doublet system (°)	0, 50, 100, 200 0, 45, 90	0 90

^aInfinite well separation is simulated by modeling only one well.

^bFor a regional flow velocity of 50 m/yr.

3.2. Sensitivity Analysis: Thermal Recovery

[25] Results of the sensitivity analysis for thermal recovery, as reached after 10 storage cycles, are shown in Figure 5. The results for horizontal correlation length (Figure 5a) show that uncertainty increases with increasing correlation length, until the correlation length is equal to the well-towell distance. For larger correlation lengths, the situation reduces to a layered subsurface and the uncertainty converges. With increasing log conductivity standard deviation (Figure 5b), the median thermal recovery decreases from 75.7% in the homogeneous case to 59.0% at a standard deviation of 2. The width of the 10/90 percentiles



Figure 4. Development of thermal recovery of the cold well during the first 10 storage and recovery cycles for the reference case (Table 2).

Table 3. The 68% Uncertainty Intervals [Helsel and Hirsch,1992] for the Relevant Statistics of the Thermal Recovery in the10th Year, for the Reference Case

P10	0.671-0.678
Median	0.692-0.706
P90	0.727-0.731
0.757	
	P10 Median P90 0.757

uncertainty range increases to 15.0 pp. Due to thermal interference (Figure 5c), thermal recovery decreases with decreasing distance between the wells. At the same time, the uncertainty related to heterogeneity increases for small well-to-well distance. At a well-to-well distance equal to one thermal radius, some of the heterogeneous realizations show slightly higher TR values than obtained for the homogeneous case. In this case, thermal interference is probably reduced due to a low hydraulic conductivity zone between the wells. Figure 5c shows that increasing the well-to-well distance beyond three R_{th} does not further increase thermal recovery or decrease uncertainty. Due to increased advective heat loss, thermal recovery declines with increasing regional flow velocity. Furthermore the uncertainty range increases from 5.2 pp in case of stagnant groundwater to 15.7 pp with a regional flow velocity of 200 m/yr (Figure 5d). The effect of the orientation of the doublet system (see Figure 2) with respect to a regional flow velocity of 50 m/yr is shown for the cold well (Figure 5e) and the warm well (Figure 5f). Here, 0° corresponds to the situation with the cold well upstream of the warm well, and 90° with the doublet perpendicular to the regional flow (Figure 2). For the situation, where the doublet is oriented parallel with the regional flow the recovery of the downstream well reduces by 8.9 pp with respect to the situation when the wells are oriented perpendicular to the regional flow. The uncertainty range increases from 7.5 to 10.5 pp.

3.3. Sensitivity Analysis: Thermal Balance

[26] The influence of heterogeneity on thermal balance is shown in Figure 6. Other than for thermal recovery, the median thermal balance for the heterogeneous simulations is similar to the homogeneous case. The median energy balance ratio (EBR) is mostly close to zero, meaning that there is no net heating or cooling of the subsurface. Only when the well doublet is at an angle to the groundwater flow direction, a systematic thermal imbalance is observed (Figure 6e). Maximum uncertainty is observed when the horizontal correlation length is equal to the well distance (Figure 6a). The uncertainty increases with increasing log conductivity standard deviation (Figure 6b) and specifically with increasing groundwater flow (Figure 6d). Because of the large spread observed in EBR for the ensemble with a flow velocity of 200 m/yr, the median value does not significantly differ from zero (at the p = 0.05 level). The effect of increasing well distance on uncertainty is small (Figure 6c).



Figure 5. Sensitivity analysis of thermal recovery (TR) after 10 storage cycles for (a) horizontal correlation length, (b) log conductivity standard deviation, (c) well-to-well distance, (d) groundwater velocity, and (e) and (f) the orientation of the doublet system with respect to the regional flow for the cold and warm well (for a groundwater flow of 50 m/yr).



Figure 6. Sensitivity analysis of the energy balance ratio (EBR) after 10 storage cycles for (a) horizontal correlation length, (b) log conductivity standard deviation, (c) well-to-well distance, (d) groundwater velocity, and (e) the orientation of the doublet system with respect to the regional flow.

3.4. Sensitivity Analysis: Apparent Dispersivity

[27] For all heterogeneous model runs in the sensitivity analysis, an apparent macrodispersivity was determined (Figure 7). The median apparent dispersivity increases with increasing log conductivity standard deviation (Figure 7b) and is relatively insensitive to changes in the other parameters. The apparent decrease in median apparent dispersivity observed at 200 m/yr (Figure 7d) with respect to the median value at 0 m/y is not significant at the p = 0.05level. As for thermal recovery, the spreading in the ensemble does not increase further when the correlation length becomes larger than the well distance (Figure 7a) and increases with increasing log conductivity standard deviation (Figure 7b), decreasing well-to-well distance (Figure 7c) and especially with increasing groundwater flow velocity (Figure 7d). The effect of the orientation of the doublet system with respect to the groundwater flow on both median and uncertainty range is small (Figures 7e and 7f).

4. Discussion

[28] From our simulations, it becomes clear that the median thermal recovery of an ATES system decreases with increasing heterogeneity (Figure 5b). Yet, when thermal interference is reduced due to a low hydraulic conductivity zone between the wells, thermal recovery in a heterogeneous aquifer can be higher than in the homogeneous aquifer, for example at small well-to-well distances (Figure 5c) or with high regional groundwater flow (Figure 5d).

[29] By comparing our results with similar model simulations for a single ATES well in a heterogeneous medium [*Ferguson*, 2007], the effect of two wells operating concurrently is illustrated. Considering two heterogeneous aquifers ($\sigma = 0.261$ and $\sigma = 1.6$), *Ferguson* [2007] also finds a reduction in the amount of extracted thermal energy with respect to the homogeneous case (respectively, 5.5% and 8.2% after one cycle). To compare our results, extracted energies are determined for every ensemble member in the first storage/recovery cycle ($\sigma = 0, 0.5, 1, 2$). Interpolating these values to $\sigma = 0.261$ and $\sigma = 1.6$ gives an average reduction of, respectively, 13.6% and 20.2%. Our simulations are more sensitive to σ , most likely due to the fact that we consider a doublet well system where preferential pathways result in energy loss due to thermal interference.

[30] Regarding the thermal balance, Figure 6 shows that the uncertainty in EBR is most sensitive to heterogeneity at the scale of the ATES system itself. For much smaller correlation lengths, the effect of hydraulic conductivity variations around the wells averages out, such that both wells are affected similarly by the heterogeneous medium. Likewise, for correlation lengths that are much larger than the scale of the ATES system, the 3-D heterogeneous medium reduces to a 2-D system consisting of homogeneous layers at the scale of the ATES system, thereby influencing the wells equally. In these cases, where both wells are affected similarly by the heterogeneous medium, EBR is close to zero (a balanced system). In a comparative study on 67 systems in Netherlands [*Koenders*, 2007] it is shown that 67% of the systems have an absolute EBR larger than 15%.



Figure 7. Sensitivity of apparent macrodispersivity after 10 storage cycles for (a) horizontal correlation length, (b) log conductivity standard deviation, (c) well-to-well distance, (d) groundwater velocity, and (e) and (f) the orientation of the doublet system with respect to the regional flow for the cold and warm well.

Considering that the groundwater flow velocity at these sites is generally below 50 m/yr and doublets are constructed preferably perpendicular to the groundwater flow, nonzero EBR observed in practice, can only for a minor part be attributed to heterogeneity. Our simulations are based on equal volumes of groundwater extracted during heating and cooling mode and fixed injection temperatures. In principle, extracted energy during heating and cooling mode could be changed individually to compensate for observed thermal imbalance during operation of the system. In contrast to this, operational ATES systems frequently experience fluctuating extraction and injection temperatures, as well as imbalances in extracted and injected groundwater volumes, in response to changing cooling and heating demands of the attached building. These changes in demand are in turn caused by changing outdoor conditions and are assumed for a large part to be responsible for ATES energy imbalances.

[31] Considering the computation time needed to perform a Monte Carlo-type simulation using heterogeneous hydraulic conductivity fields, it would be convenient to express the effect of heterogeneity in a single, a priori determined parameter such as macrodispersivity, enabling the use of homogeneous models. Analytical solutions for the relationship between macrodispersivity and heterogeneity have been derived for both solute transport [*Attinger et al.*, 2001; *Gelhar*, 1993; *Hsu*, 2003] and heat transport [*Chang and Yeh*, 2012]. The solutions differ in the method that is used to derive them (e.g., homogenization/spectral analysis) and the assumptions used (e.g., parallel/radial flow fields, isotropic/anisotropic conditions, spatial correlation function and in-/or excluding diffusion and local dispersivity). Although no solution was found that exactly matches the conditions of our simulations, a comparison is presented here to illustrate the specific features for the case of an ATES system.

[32] A comparison is provided with the solutions of Attinger et al. [2001]. Chang and Yeh [2012], and Gelhar [1993] for which formula and main assumptions are given in Appendix A. The numerical solutions are all derived for large displacement conditions $(\int q/n \cdot dt \gg \lambda_h)$, whereas in our case the transported distance is of the same order of magnitude as the correlation length (λ_h) . Since local temperature differences do not average out at this length scale, we observe an uncertainty in thermal recovery which calls for a range in macrodispersivity values instead of a single value. The solutions in Chang and Yeh and Gelhar are derived for isotropic conditions. For these cases our numerical results are compared with the analytically derived apparent macrodispersivity for both the horizontal correlation length $(2 \cdot R_{th})$, 104.1 m for the reference case; Figure 8a) and the vertical correlation length (2 m; Figure 8b) as used in our simulations. As the main flow direction is in the horizontal plane, the first (horizontal comparison) could be considered as most relevant. However, using either the anisotropic solution of Attinger et al. or the horizontal correlation length in the isotropic solutions of Chang and Yeh and Gelhar, these analytical solutions calculate much higher dispersivity values than the apparent macrodispersivities found in this



Figure 8. Comparison of numerical results for macrodispersivity with closed-form analytical solutions. *Gelhar* [1993] and *Chang and Yeh* [2012] are derived for isotropic conditions. These solutions are calculated using (a) the horizontal correlation length (104.1 m) and (b) the vertical correlation length (2 m) as used in this study. Note that in Figure 8a the Chang and Yeh solution results in a steep curve near the *y* axis. The solution from *Attinger et al.* [2001] is derived for anisotropic conditions and is calculated using $\lambda_v = 2 \text{ m}$ and $\lambda_h = 104.1 \text{ m}$.

study. On the other hand, the small vertical correlation length could generate preferential pathways and thereby promote the tendency for horizontal interaction between the wells. Using the vertical correlation length in the solutions of Chang and Yeh and Gelhar results in similar dispersivity values as found in this study. We can, however, not show if this is also true for other ratios between $\lambda_{\rm h}$ and $\lambda_{\rm v}$.

[33] In previous studies [Ferguson, 2007; Hidalgo et al., 2009; Vandenbohede et al., 2009] it has been suggested that thermal diffusion is able to smooth temperature differences due to preferential flow and thereby reduce the effect of heterogeneity. This concept is tested by comparing the magnitude of thermal conduction with the expected size of temperature fluctuations due to heterogeneity. In the modeled scenarios, as in most actual aquifers, the horizontal correlation length is much larger than the vertical correlation length [Gelhar, 1993]. Comparison of vertical diffusion time $(\tau = \lambda_v^2/D_{th} = 10.5 \text{ days})$ with the average residence time (182.5 days for one storage cycle) shows that there is ample time for thermal diffusion to level out temperature differences due to preferential flow, resulting in a macrodispersivity only slightly larger than the local dispersivity. Because the diffusion coefficient for heat, $0.382 \text{ m}^2/\text{d}$ (Table 1), is several orders of magnitude larger than for chemical tracers like Cl^{-} (1.4E-5 m²/d) [*Fitts*, 2002; Li and Gregory, 1974], this effect is much stronger in the case of heat transport than for solute transport. Running our simulations for nonreactive solute tracer transport, showed more distinctive fingering and increased spreading of the tracer front than in the case of heat transport (animations of the evolution of temperature as well as tracer concentrations around the wells are attached as auxiliary material; simulation results are provided as horizontal and vertical cross sections for the homogeneous case and one heterogeneous case ($\lambda = 2 R_{th}, \sigma = 2$, well distance = 2 R_{th} , regional groundwater velocity = 0 m/yr).

[34] A second difference between our case and the conditions used in deriving the analytical solutions for macrodispersivity is that the injected heat is extracted back over the same flow paths. In this case, the dispersive effect of heterogeneity is partly reversed while extracting (i.e., the more permeable parts that transported heat more effectively during injection also transport it back when extracting), also resulting in a lower value for macrodispersivity. A last important difference between the analytical solutions and our simulations is that we consider the flow field around a dipole well system. Where for a single well, flow and advective transport are reversible, this is not the case in a doublet well system. Due to thermal interference, stored energy that reaches the other well is not extracted. Because of thermal interference, apparent macrodispersivity for a doublet well system does not depend only on the statistical and actual properties of the subsurface, but also on well-to-well distance and the configuration of the wells (Figure 7).

4. Conclusions

[35] Heterogeneity in hydraulic conductivity affects the distribution of thermal energy around ATES systems. This in turn has an effect on the thermal recovery and the thermal balance of the system. Using a Monte Carlo approach, the sensitivity of ATES performance to heterogeneity was determined. Simulations of a doublet well system, with a well-to-well distance equal to two thermal radii, show that the median thermal recovery in moderately heterogeneous media (log conductivity standard deviation of 1-2) is 6-15 percent point (pp) lower than in a homogeneous medium. Even without significant regional groundwater flow, uncertainty in the degree of thermal interference for heterogeneous aquifers results in an uncertainty in predicted thermal recovery up to 15 pp.

[36] In regulations for ATES, balanced conditions are important, which means a volume balance and equal temperature offset between the warm and cold well and the natural aquifer temperature. When the ATES system is operated under such conditions, sensitivity of the energy balance to heterogeneity is only minor. All modeled cases with a regional groundwater flow of less than 50 m/yr show an absolute energy balance ratio smaller than 4%. However, in the case of high regional groundwater flow uncertainty in expected EBR is larger (up to 22% for a flow velocity of 200 m/yr).

[37] The results indicate that it is possible to capture the effect of heterogeneity on thermal recovery in homogeneous models by applying a range of macrodispersivities. However, the appropriate range of dispersivities not only depends on the correlation length and log conductivity standard deviation, but also on groundwater velocity and well-to-well distance.

[38] Considering the increasing demand for ATES systems, we conclude that thermal interference limits the number of ATES systems that can be built in a specific area. Furthermore, uncertainty in the hydraulic conductivity field related to heterogeneity should be accounted for when optimizing well-to-well distance for the wells within a single system and between systems. This study is limited to thermal interference between two wells and the effect of heterogeneity on the performance of a single doublet well ATES system. ATES performance reduction due to interference in regional, multisystem situations might be partly compensated by interference between wells with similar temperature [*Bakr et al.*, 2013].

Appendix A: Closed-Form Solutions of Macrodispersivity as a Function of Correlation Length (λ) and Log Conductivity Standard Deviation (σ)

- [39] *Gelhar* [1993]
- [40] Main assumptions:
- [41] 1. Isotropic log conductivity field.
- [42] 2. Steady parallel flow field.
- [43] 3. Including local dispersive mixing (no diffusion).
- [44] 4. Ideal tracer conditions (nonreactive solute and constant density and viscosity).
 - [45] 5. Transport scale >> correlation length.

[46] Formula [modified from *Gelhar*, 1993, equation 5.2.13, p. 221]:

$$\alpha_{L,app} = \sigma^2 \lambda / e^{\sigma^2/3} \tag{A1}$$

- [47] $\alpha_{L,app}$, longitudinal macrodispersivity;
- [48] σ , log conductivity standard deviation;
- [49] λ , correlation length.
- [50] Attinger et al. [2001]
- [51] Main assumptions:
- [52] 1. Anisotropic Gaussian correlation function.
- [53] 2. Steady radially diverging flow field.
- [54] 3. Including vertical diffusion (no dispersion).

[55] 4. Ideal tracer conditions (nonreactive solute and constant density and viscosity).

- [56] 5. Transport scale >> correlation length.
- [57] Formula [modified from *Attinger et al.*, 2001, equation 51]:

$$\alpha_{L,app} = \sigma^2 \lambda_h \int_0^{r/\lambda_h} e^{-\hat{r}^2} / \sqrt{1 + \frac{Dn\lambda_h^2}{Q\lambda_v^2} \left(r/\lambda_h \hat{r} - \hat{r}^2/2\right)} \cdot d\hat{r} \quad (A2)$$

- [58] $\alpha_{L,app}$, longitudinal macrodispersivity.
- [59] σ , log conductivity standard deviation;
- [60] λ_h , horizontal correlation length;
- [61] λ_{ν} , vertical correlation length;
- [62] D, (thermal) diffusion coefficient;
- [63] *Q*, discharge of the well/meter of well screen;
- [64] n, porosity;
- [65] r, radial distance.
- [66] Chang and Yeh [2012]
- [67] Main assumptions:
- [68] 1. Isotropic Gaussian log conductivity field;
- [69] 2. Steady parallel flow field;
- [70] 3. Including diffusion (no dispersion);
- [71] 4. Constant density and viscosity;
- [72] Formula [*Chang and Yeh*, 2012, equation 24]:

$$v = \rho_w c_w / (\rho_a c_a)$$

$$\eta = \sqrt{P\tau^2 / (P + 4\tau)}$$

$$q = Q / (2\pi r)$$

- [73] $\alpha_{L,app}$, longitudinal macrodispersivity;
- [74] σ , log conductivity standard deviation;
- [75] λ , correlation length;
- [76] *D*, (thermal) diffusion coefficient;
- [77] *Q*, discharge of the well/meter of well screen;
- [78] q, specific discharge;
- [79] *r*, radial distance to the well;
- [80] ρ_{w} , density of water;
- [81] c_w heat capacity of water;
- [82] ρ_a density of aquifer;
- [83] c_a , heat capacity of aquifer;
- [84] k_{a} , thermal conductivity of aquifer;
- [85] φ , error function;
- [86] ψ , complementary error function.

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