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Highlights

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- Heterogeneity has a relevant impact on geothermal system efficiency.
- Heterogeneity of hydraulic conductivity affects the transient of thermal feedback.
- Heterogeneity and dispersivity do not affect long-term behaviour of well doublets.
- Uncertainty increases with medium heterogeneity in non-ergodic conditions.

The impact of porous medium heterogeneity on the thermal feedback of open-loop shallow geothermal systems

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Abstract

Groundwater has been increasingly used to provide low-carbon heating and cooling of buildings with open-loop shallow geothermal systems. Water is generally reinjected into the same aquifer after the heat exchange in order to avoid the aquifer depletion. However, this can result in the return of part of the injected water to the production well(s), causing a gradual thermal alteration known as thermal feedback. Thermal feedback is a major design issue of open-loop shallow systems but, so far, it has been mainly addressed neglecting the heterogeneity of the aquifer properties. This study investigates the impact of aquifer heterogeneity on two main metrics that characterize thermal feedback: thermal breakthrough time (i.e., the first arrival time of the thermal plume) and recirculating ratio (i.e., the fraction of water coming back to production well). A stochastic approach was adopted performing a large number of numerical simulations that cover a wide range of possible scenarios. Results highlight that conductivity heterogeneity plays a major influence on the temperature evolution at the production well. The breakthrough time alone might lead to misleading evaluations of the system efficiency, given that a few particles can reach the production well by traveling in the highly-conductive layers. Conversely, both the heterogeneity and the thermal dispersivity have a negligible impact on the recirculating ratio, which quantifies the long-term evolution of thermal feedback. As a consequence, the available approaches based on advection-only and homogeneous medium are a robust tool to predict the long-term behaviour of shallow open-loop geothermal systems.

Keywords: Geothermal systems, Thermal feedback, Thermal breakthrough time, Stochastic

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1 **1. Introduction**

2 The use of shallow geothermal energy for heating and cooling of buildings has become popular
 3 thanks to the low operational costs and the low carbon intensity (Casasso and Sethi, 2019; Bayer
 4 et al., 2019; Lund and Toth, 2020; Tissen et al., 2021; Bartolini et al., 2020). The heat in the
 5 subsurface can be exploited by shallow geothermal systems in two ways: through the circulation
 6 of a heat carrier fluid into a closed pipe loop (closed-loop systems) or by exchanging heat
 7 with groundwater (open-loop systems). Generally speaking, closed-loop systems are installed in
 8 the absence of an exploitable aquifer or, for small-power installations (e.g., below 100 kW),
 9 to avoid the maintenance issues typical of wells. Open-loop systems are more popular for
 10 large-scale installations up to a few MW thanks to their higher efficiency and the economies
 11 of scale (Tsagarakis et al., 2020). Large flow rates in the order of tens or even hundreds of L/s
 12 are abstracted to provide such a large thermal power and, for this reason, water is generally
 13 reinjected into the same aquifer to avoid its depletion and depressurization (Horne, 1985; Banks,
 14 2012).

15 However, reinjection raises a few possible issues, among which the return to the production
 16 well(s) of a share of the reinjected water (Milnes and Perrochet, 2013). Since the temperature of
 17 reinjected water is different from the background value of the aquifer (i.e., colder when the plant
 18 operates in heating mode, and hotter when it operates in cooling mode), the abstracted water
 19 progressively decreases or increases its temperature. Such a process occurs at the production
 20 well only under certain hydraulic conditions, which are seldomly avoidable in densely-populated
 21 urban areas (Clyde and Madabhushi, 1983; Kong et al., 2017). The gradual thermal alteration
 22 of abstracted water is defined *thermal feedback* or *thermal recycling* according to the operat-
 23 ing parameter imposed, that is, respectively, the reinjection temperature or the temperature
 24 difference between reinjected and abstracted water (Milnes and Perrochet, 2013). This study
 25 adopts constant reinjection temperatures and therefore focuses on the issues related to thermal
 26 feedback, which might gradually compromise the efficiency of the geothermal plant even to its
 27 failure (Banks, 2009). In order to prevent this, the temperature of reinjected water has a min-
 28 imum and a maximum limit. The minimum temperature allowed is, theoretically, the water
 29 icing (0°C); however, a safety margin must be imposed on this value. The maximum tempera-

30 ture allowed depends on technical constraints, such as the operating limits imposed by the heat
31 pump manufacturer or the HVAC (Heating, Ventilation, and Air Conditioning) designer and
32 on legislative constraints. Indeed, reinjection of warm water has several potentially negative
33 impacts on groundwater ecosystems and on groundwater quality (Casasso and Sethi, 2019), as
34 well as on neighbouring and downstream shallow geothermal installations (Epting et al., 2017;
35 Barla et al., 2018; Pophillat et al., 2020).

36 Thermal feedback is therefore a major design issue for open-loop shallow geothermal systems.
37 So far, the literature addressed this issue mainly considering a homogeneous porous medium.
38 Early publications (Gringarten and Sauty, 1975; Lippmann and Tsang, 1980) and more recent
39 works (Luo and Kitanidis, 2004; Milnes and Perrochet, 2013; Kong et al., 2017) provided the
40 mathematical framework to address thermal feedback under the following assumptions: i) homo-
41 geneous porous medium, ii) constant operating conditions (flow rate, temperature difference),
42 and iii) a well doublet aligned with groundwater flow. Recently, Casasso and Sethi (2015) de-
43 veloped a MATLAB code to assess thermal feedback with arbitrary well doublet alignments and
44 derived an empirical formula to estimate the time trend of well temperatures for wells aligned
45 with groundwater flow.

46 However, solutions based on homogeneous conductivity and effective macrodispersion coef-
47 ficients are not able to grasp the effect of aquifer heterogeneity on thermal plume dynamics.
48 Since the traditional procedures assuming homogeneous conductivity might lead to an incorrect
49 design or an erroneous interpretation of the plant performance, we shall consider a stochas-
50 tic approach (Dagan, 1989; Rubin, 2003; Fiori et al., 2015a; Kitanidis, 2015) to evaluate the
51 effect of heterogeneity on shallow geothermal systems. By increasing the conductivity hetero-
52 geneity, preferential flow paths emerge, thereby altering the temperature distribution at the
53 production well (Pandey et al., 2018). Moreover, data scarcity does not allow a highly detailed
54 description of the spatial variability of conductivity (Nowak et al., 2010; Maya et al., 2018).
55 Consequently, such a lack of knowledge leads to high uncertainty in the predicted values. More
56 precisely, heterogeneity in hydraulic conductivity could significantly affect the metrics used to
57 evaluate the efficiency of geothermal systems. One of the most considered metrics is the *thermal*
58 *breakthrough time* (Clyde and Madabhushi, 1983), which is defined as the first arrival time of a
59 thermal plume travelling back to the production well and is ruled by the flow patterns in the well
60 doublet. Another metric is the *recirculating ratio*, which quantifies the fraction of the injected

61 water returning to the production well and it is an indicator of the long-term sustainability of
62 the system (Milnes and Perrochet, 2013).

63 So far, a small number of studies have investigated the impact of heterogeneity on the
64 geothermal systems. Liu et al. (2019) examined the response of a well pair system in a heteroge-
65 neous geothermal reservoir during continuous time operation. They studied how the variability
66 of hydraulic conductivity, heat capacity and correlation length affect the well pair performances.
67 They showed that breakthrough time decreases with increasing heterogeneity degree and cor-
68 relation length values. Babaei and Nick (2019) addressed low-enthalpy well doublets with an
69 initial temperature of 75°C and a reinjection at 30°C. In particular, they hypothesized a hetero-
70 geneous and spatially correlated porosity field (assessing the effect of different values of variance
71 and correlation length) and a permeability field that varies accordingly. They found that an
72 increase of variance and/or correlation length of the porosity (and, hence, permeability) results
73 in a decrease of the well doublet lifetime, defined as the time it takes for the abstracted water
74 temperature to be reduced by 1°C. The same lifetime definition was previously used by Crooi-
75 jmans et al. (2016) and by Willems et al. (2017) for a sedimentary fluvial reservoir considering
76 different facies realizations. Watanabe et al. (2010), on the other hand, modelled a Hot Dry
77 Rock reservoir with an equivalent porous medium approach, focusing on the propagation of the
78 thermal plume downstream the reinjection well. They found that this phenomenon is mostly
79 influenced by permeability and, to a lesser extent, by the thermal capacity, whereas the thermal
80 conductivity has a negligible influence. The aforementioned studies focused on deep geothermal
81 systems, which are generally characterized by low intrinsic permeabilities (10^{-18} - 10^{-12} m² accord-
82 ing to Moeck (2014)) and large temperature differences between abstraction and reinjection, i.e.,
83 in the order of tens of centigrade degrees. Shallow open-loop geothermal systems are installed in
84 more permeable formations (10^{-11} - 10^{-9} m² according to Sethi and Di Molfetta (2019)) and adopt
85 temperature differences within a few degrees (e.g., ± 4 K according to Casasso et al. (2020)).
86 To the authors' knowledge, so far no study has addressed the impact of the heterogeneity of
87 subsurface properties on the operation of shallow open-loop geothermal systems.

88 The aim of this work is to test the impact of hydraulic conductivity heterogeneity on heat
89 transport in open-loop shallow systems through a stochastic modelling framework. Our objec-
90 tives are the following:

- 91 • Focusing on the interplay between heterogeneity and several thermo-hydro-geological pa-

92 parameters (e.g. thermal diffusion or pore-scale dispersivity) and engineering parameters
93 (e.g., wells arrangement or operational pumping rates).

- 94 • Analyzing the behavior of the breakthrough time, i.e. the shortest time a water particle
95 employs to move from the injection to the extraction well, and the recirculating ratio as a
96 function of the main design parameters.
- 97 • Comparing the numerical results with the analytical solutions available in literature, in
98 order to test the potentialities and limitations of more simplified approaches.
- 99 • Assessing the uncertainty due to the limited knowledge of the subsurface characterization
100 and its effect on the system performance.

101 The paper is structured as follows. Section 2 presents the methodology by describing the
102 thermal feedback problem, the theoretical framework of heat transport in heterogeneous porous
103 media, and the numerical modelling setup. Section 3 presents the results divided into the analysis
104 of the thermal breakthrough time, the recirculating ratio, the temperature at the pumping
105 well and the ergodicity issue, discussing the main findings and the relationship with existing
106 literature. Conclusions are reported in Section 4.

107 **2. Methodology**

108 *2.1. Problem statement*

109 In this work we consider an open-loop shallow geothermal system for the heating of buildings
110 (though the same approach can also be applied to a cooling plant). The geothermal system
111 consists of a well doublet placed into a confined aquifer of constant thickness B . A uniform-in-
112 the-mean regional flow crosses the aquifer. Assuming a system of reference $\mathbf{x} = \{x_1, x_2, x_3\}$, the
113 regional flow is aligned to x_1 . Groundwater is abstracted upstream and, after the heat exchange,
114 it is reinjected downstream with a constant lower temperature. The angle between the regional
115 flow and the well doublet is defined as θ and it is measured as shown in Figure 1. The wells in
116 the doublet are placed at a distance L . The two wells are working at a constant rate Q_w , so
117 that the model is steady-state for flow and transient for heat transport.

118 The pumping activity modifies the natural flow field and determines a local inversion of
119 groundwater flow in the zone between the two wells. If the injected water reaches the extrac-
120 tion well, we have the so called *thermal feedback*, which determines a progressive alteration of

121 the water temperature at the production well T_{prod} with a consequent decrease of the system
 122 efficiency. The occurrence of the thermal feedback depends on hydrogeological characteristics,
 123 such as the hydraulic conductivity K , the regional-flow gradient $\mathbf{J} = \{J, 0, 0\}$ and the aquifer
 124 depth B , as well as engineering parameters, such as the pumping rate Q_w and the wells spatial
 125 arrangement (i.e. the well distance L and the angle θ).

126 This problem can be studied by interpreting heat as a tracer moving in a porous medium.
 127 Such an assumption is valid under Local Thermal Equilibrium (LTE) between the rock and
 128 the fluid (Shook, 2001; Hoehn and Cirpka, 2006; Markle and Schincariol, 2007; Hecht-Méndez
 129 et al., 2010; Stauffer et al., 2019; Irvine et al., 2015; Sarris et al., 2018; Gossler et al., 2019).
 130 As a consequence, the thermal plume moves through both pores and soil matrix and thus it
 131 is slower than the fluid velocity. The thermal retardation factor R_{th} can be quantified as the
 132 ratio between the thermal capacity of the porous medium and the thermal capacity of water, as
 133 follows (Shook, 2001):

$$R_{th} = \frac{\rho_s c_s}{n \rho_w c_w} \quad (1)$$

134 where ρ_w and ρ_s are the water and the solid matrix densities, respectively, c_w and c_s the specific
 135 heat capacities of water and solid matrix, respectively, and n is the porosity.

136 The thermal breakthrough time τ_0 , namely the shortest time a water particle spends travel-
 137 ling from the injection well to the production well, is the metric commonly adopted to evaluate
 138 the thermal feedback. So far, most of practical studies (Gringarten and Sauty, 1975; Lippmann
 139 and Tsang, 1980; Clyde and Madabhushi, 1983; Milnes and Perrochet, 2013; Casasso and Sethi,
 140 2015) have evaluated τ_0 by means of a closed analytical solution that assumes a homogeneous
 141 domain, a mean regional flow aligned with the pumping wells (i.e. $\theta = 0$) and advective-
 142 only transport. Under such hypotheses the analytical breakthrough time τ_0^{an} can be calculated
 143 through the complex potential theory as follows (see, e.g., Strack, 2017; Luo and Kitanidis,
 144 2004):

$$\tau_0^{an} = R_{th} \frac{nL}{KJ} \left[\frac{\chi}{\sqrt{\chi-1}} \tan^{-1} \left(\frac{1}{\sqrt{\chi-1}} \right) - 1 \right] \quad (2)$$

145 where χ is the dimensionless pumping rate

$$\chi = \frac{2Q_w}{\pi BKJL} \quad (3)$$

146 Providing that the aforementioned assumptions are satisfied, the thermal feedback occurs only
 147 when $\chi > 1$ (Luo and Kitanidis, 2004).

148 In order to evaluate the sustainability of an open-loop system, designers also need to quantify
 149 the long-term effect. A typical metric is the fraction of injected water returning to the production
 150 well RR , which provides the indication of the efficiency decay of the plant. As well as for τ_0^{an} ,
 151 a closed form analytical solution can be introduced to assess RR^{an} under the assumption of
 152 advective transport and well doublet aligned with the mean flow (Milnes and Perrochet, 2013):

$$RR^{an} = \frac{2}{\pi} \left[\tan^{-1} \left(\sqrt{\chi - 1} \right) - \frac{\sqrt{\chi - 1}}{\chi} \right] \quad (4)$$

153 We emphasize that these analytical formulae (e.g. eqs. (2) and (4)) are obtained assuming
 154 only convective heat transport, neglecting conduction, medium heterogeneity and other pore-
 155 scale dispersive/diffusive phenomena. Introducing these more realistic phenomena or angle θ
 156 different from zero requires the use of numerical solution schemes. Moreover, these solutions
 157 neglect the spreading of the flow trajectories operated by the natural heterogeneity of real
 158 aquifers. Heterogeneity determines the emergence of fast flow paths and stagnation zones in the
 159 medium, thereby exerting a significant impact on τ_0 (Wen and Gómez-Hernández, 1996; Zinn
 160 and Harvey, 2003; Knudby and Carrera, 2006; Fiori and Jankovic, 2012). Given that in the
 161 ergodic case τ_0 assumes values in the range $(0, +\infty)$, a significant deviation from the equivalent
 162 homogeneous solution is expected in heterogeneous media. In the next sections, we present
 163 the mathematical framework and the numerical setup to study open-loop shallow systems in
 164 heterogeneous porous media.

165 2.2. Theoretical framework

166 Figure 1 depicts a sketch of the conceptual model considered here. We assumed that the
 167 flow field occurs in a 3-D confined and stratified aquifer, which is made of N layers, each one
 168 characterized by a random homogeneous hydraulic conductivity K_i , for $i = 1, N$. The log-
 169 conductivity field $Y = \ln K$ is modeled as a stationary random variable normally distributed
 170 with mean $\ln(K_G)$, with K_G the geometric mean of K , and variance σ_Y^2 (Freeze, 1975; Fiori
 171 et al., 2015b). The thickness of each layer is $2I_v$, with I_v the vertical integral scale of Y , such
 172 that the number of layers is $N = B/(2I_v)$. Water is injected over the total thickness of the
 173 aquifer, in such a way that each layer conveys a flux proportional to the local K_i (see, e.g.,

174 Kreft and Zuber, 1978; Demmy et al., 1999; Frampton and Cvetkovic, 2009). This stratified-
 175 formation conceptual scheme is quite common in groundwater studies dealing with contaminant
 176 migration in groundwater (e.g. Zavala-Sanchez et al., 2009; Pedretti and Fiori, 2013; Zech et al.,
 177 2018) and can be considered suitable for systems with $L < I_h$, with I_h the Y horizontal integral
 178 scale.

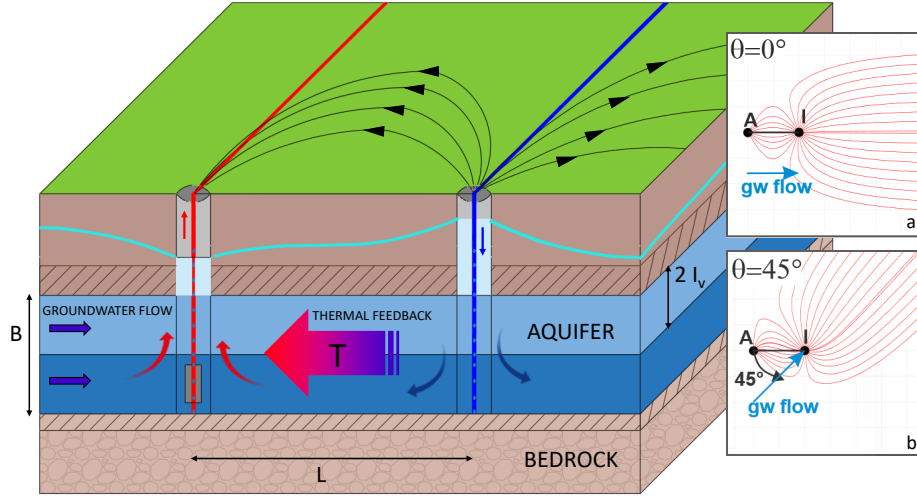


Figure 1: A sketch of the conceptual model. The porous formation is a 3-D confined and stratified aquifer. It is composed of a series of N layers of conductivity K_i , with $i = 1, N$. The conductivity is a stationary random variable lognormally distributed. A well doublet operating as a geothermal system is placed at the center of the domain. Insets a and b show two configurations of the angle θ between the wells and the regional flow.

179 At the beginning of the simulation, groundwater is at a constant temperature T_{ref} . After
 180 being extracted from the production well, water is reinjected in the injection well at a different
 181 temperature T_{well} . As a consequence, a heat plume develops from the injection well, and part of
 182 this flow can reach the production well located upstream. Heat transport in geothermal system
 183 results from the interplay of different physical phenomena such as conduction, thermal advec-
 184 tion and thermal dispersion (Carslaw and Jaeger, 1959). Conduction is the direct microscopic
 185 transfer of kinetic energy between atoms and molecules. It results in heat moving in the opposite
 186 direction of temperature gradient. Thermal advection is the transport of heat due to the motion
 187 of a fluid moving from one place to another. Thermal dispersion is the heat exchange occur-
 188 ring in porous media due to the nonuniformity in temperature and velocity at the pore-scale

189 (Özgümüş et al., 2013).

190 Under LTE, heat transport in porous media can be modelled in a similar way to the transport
191 of solutes. Thus at the Darcy-scale, heat transport can be described by the advection-dispersion
192 equation for solute transport (De Marsily, 1986):

$$-\nabla \left(\frac{\mathbf{q}}{n} T \right) + \nabla (D \nabla T) + \frac{q_H}{n \rho_w c_w} = R_{th} \frac{\partial T}{\partial t} \quad (5)$$

193 where T is the local temperature, q_H the heat source, \mathbf{q} the water flux at the Darcy-scale, related
194 to advection, and D is the thermal dispersion which accounts for the heat transfer at pore scale.
195 The thermal dispersion D is given by the sum of two different components, the thermal diffusion
196 D_{th} and the pore-scale dispersion D_α :

$$D = D_{th} + D_\alpha = \frac{\lambda}{n \rho_w c_w} + \alpha_d \frac{|\mathbf{q}|}{n} \quad (6)$$

197 where λ is the effective thermal conductivity of the medium, α_d the pore-scale dispersivity, here
198 assumed as isotropic, and $|\mathbf{q}|$ is the magnitude of the local velocity. The water flux can be
199 described by the well known Darcy equation:

$$\mathbf{q} = -K \nabla \phi = -K \mathbf{J} \quad (7)$$

200 where ϕ is the hydraulic head.

201 Eq. (5) assumes constant water density and viscosity, thus neglecting the temperature
202 dependence on these properties. The limited temperature ranges at which shallow geothermal
203 systems operate (i.e., up to $\pm 6^\circ\text{C}$ compared to background temperature) induce a slight variation
204 of water properties that makes this assumption plausible, as reported in Hecht-Méndez et al.
205 (2010). Under such hypotheses, eq. (5) is formally identical to the *advection dispersion equation*,
206 which describes the solute migration of a sorbing solute in groundwater (Shook, 2001; Hidalgo
207 et al., 2009). By taking advantage of such a mathematical and conceptual equivalence, transport
208 is simulated with a particle tracking procedure developed along a Lagrangian framework. This
209 approach has been extensively used and tested in studies dealing with the solute transport in
210 heterogeneous aquifers with several levels of complexity (Cortis and Berkowitz, 2005; Salamon
211 et al., 2006; Rizzo et al., 2019).

212 The procedure adopted here is the equivalent random walk formulation of eq. (5), which
 213 aims to mimic the water and heat transport in the domain (Kinzelbach, 1988; Uffink, 1988). We
 214 consider a water parcel which, once released in the injection well with temperature T_{well} , moves
 215 in the flow domain following a flow path. The “total” trajectory $\mathbf{X}(t)$ of the water parcel can be
 216 written as the sum of two independent components: i) the advective one related to the Darcy-
 217 scale advective velocity, and ii) the fluctuation component $\mathbf{X}'(t)$ which represents phenomena
 218 acting at the pore or microscopic scale. The fluctuation, which summarizes the effects of pore-
 219 scale dispersion and conduction, is described here by a Wiener process characterized by the local
 220 dispersion coefficient $D = D_{th} + D_{\alpha}$ (see eq. (6)). In the following, we shall adopt for simplicity
 221 an isotropic pore-scale tensor. The total trajectory $\mathbf{X}(t)$ can be written as:

$$\mathbf{X}(t) = \mathbf{X}_0 + \int_0^t \mathbf{v}(\mathbf{x}, t - \tau) d\tau + \mathbf{X}' \quad (8)$$

222 with \mathbf{X}_0 the initial position of the particle and

$$\mathbf{X}' \in N[0, 2Dt/R_{th}] \quad (9)$$

223 where $\mathbf{v}(\mathbf{x}, t) = \mathbf{q}(\mathbf{x}, t)/(n R_{th})$ is the local Darcy-scale advective velocity in the position \mathbf{x} at
 224 time t . The dispersion term plays a key role: it determines the deviation of the water particles
 225 from the advective streamlines, thereby triggering mixing, macrodispersion and heat dispersion
 226 phenomena (Rubin et al., 1999; Shook, 2001; Villiermaux, 2012; Le Borgne et al., 2013; Dentz and
 227 de Barros, 2015; Di Dato et al., 2018). Given that the heat transport occurs along the flow paths,
 228 their ensemble constitutes the heat plume, namely the portion of the domain with temperature
 229 affected by the heat injection. Since the temperature is regarded as a tracer associated to the
 230 water particles, its assessment in a given position of the flow field would require an ensemble
 231 average over different realizations. However T_{prod} at the extraction well can be obtained by
 232 taking the average over the flow paths entering in the well and invoking the ergodicity (Dagan,
 233 1991).

234 In this work we adopt a numerical scheme for the Lagrangian particle tracking procedure.
 235 Beside the two lumped parameters τ_0 and RR , we analyze the temperature evolution at the
 236 production well. In fact, although the two metrics τ_0 and RR can be used for a fast assessment
 237 of the geothermic plant efficiency, they do not give any information on the temperature evolution
 238 at the production well, which in turn assesses the plant efficiency evolution in time.

239 *2.3. Numerical setup*

240 On the line of the theoretical framework discussed in the previous section, we developed
 241 a numerical code to investigate how spatial heterogeneity, thermal dispersion and engineering
 242 parameters affect the thermal feedback metrics, i.e. τ_0 and RR , and the temperature evolution at
 243 the production well. The flow field is solved by means of the finite volume scheme of MODFLOW-
 244 2005 (Harbaugh, 2005), which is managed through the FloPy python script (Bakker et al., 2016).
 245 The thermal propagation is modelled by following the Lagrangian approach through the particle
 246 tracking procedure outlined in Di Dato et al. (2019). The injected mass is modelled with a cloud
 247 of particles and transport is simulated by tracking them according to the Itô–Taylor integration
 248 scheme (Itô, 1951):

$$\mathbf{X}_p(t + \Delta t) = \mathbf{X}_p(t) + \mathbf{A}(\mathbf{X}_p, t)\Delta t + \mathbf{B}(\mathbf{X}_p, t) \epsilon \sqrt{\Delta t} \quad (10)$$

249 where \mathbf{X}_p is the particle position at the initial time t , Δt is the numerical time step, ϵ is a vector
 250 of independent normally distributed random numbers with zero mean and unit variance and the
 251 tensors \mathbf{A} and \mathbf{B} are defined, respectively, as (Kinzelbach, 1988; Uffink, 1988):

$$\mathbf{A} = \mathbf{v} + \nabla \cdot \left(\frac{D}{R_{th}} \right) \mathbf{I} \quad (11)$$

$$\mathbf{B} \cdot \mathbf{B}^T = \left(2 \frac{D}{R_{th}} \right) \mathbf{I} \quad (12)$$

252 where \mathbf{I} is the identity tensor. The time step Δt is chosen by following the particle tracking
 253 procedure outlined in Di Dato et al. (2019, see Appendix A). The authors proposed a modified
 254 version of the algorithm of Pollock (1988) to model diffusion and pore-scale dispersion. Di Dato
 255 et al. (2019) verified the accuracy of their algorithm by comparing the numerical results with a
 256 3rd order Runge-Kutta scheme (Drummond et al., 1984) and the analytical solution of Moench
 257 (1989) obtaining a very good match.

258 As the focus of this paper is on the production of shallow geothermal energy for heating
 259 and cooling of buildings, the system domain is chosen to model the typical size of a small
 260 installation, e.g. for a detached house, in which the available space for well distancing is not
 261 large. The numerical domain depicts a perfectly stratified porous medium with a constant
 262 depth $B = 10$ m divided in 10 layers of thickness equal to $2I_v = 1$ m. Such a value of I_v

263 is consistent with the values encountered in natural porous formations (Rubin, 2003). Each
 264 layer is homogeneous and characterized by a random log-conductivity $Y = \ln K$ drawn from a
 265 normal distribution with mean $\ln(K_G)$ and variance σ_Y^2 . In stratified media the geometric mean
 266 is given by $K_G = K_{eff}/\exp(\sigma_Y^2/2)$, where the effective conductivity K_{eff} is equivalent to the
 267 arithmetic mean of K . We stress that here the definition of K_{eff} refers to a system subject only
 268 to regional flow and it is not a property of strongly nonuniform well flow (Bellin et al., 2020).
 269 The dimensionless pumping rate χ in heterogeneous media is therefore defined as:

$$\chi = \frac{2Q_w}{\pi BK_{eff}JL} \quad (13)$$

270 We explore three heterogeneous scenarios ranging from homogeneous ($\sigma_Y^2 = 0$) to mild hetero-
 271 geneity degree, i.e. $\sigma_Y^2 = 1$ and 2.

272 Two fixed heads are assigned to the left and the right boundaries, such that a regional
 273 flux develops from left to right. In order to model a confined aquifer, the hydraulic heads
 274 are set higher than the aquifer top. Two wells are located at the center of the computational
 275 domain at a distance of $L = 10$ m and the line joining the wells forms an angle of θ with
 276 the regional flux. As stated in Casasso and Sethi (2015), the convention adopted is that θ
 277 is measured counterclockwise from the line joining the wells. The upstream well is extracting
 278 and the downstream one is injecting water at equal constant rate Q_w , in such a way to create
 279 an open loop. Three setups are considered here: $\theta = 0, \pi/4$ and $\pi/2$. The pumping rate is
 280 chosen in such a way to investigate χ ranging from 2 to 12. The 3-D computational grid is
 281 $7L \times 7L = 70 \text{ m} \times 70 \text{ m}$ in the horizontal direction, which suffices to avoid the well influence at
 282 the boundaries. The dimensions of the computational cell are $L/50 = 0.2$ m on the horizontal
 283 direction and $I_v/4 = 0.125$ m on the vertical direction.

284 The thermal dispersion is given by the sum of the thermal diffusion D_{th} and pore-scale
 285 dispersion D_α , as defined by eq. (6). We consider here four scenarios, given by the combination
 286 of $\alpha_d = 0$ and 0.001 m (Fiori and Dagan, 1999) and $D_{th} = 0$ and $10^{-6} \text{ m}^2/\text{s}$ (Holman, 2008,
 287 Appendix A, Table A-3), which grasp the range of values typically observed in natural aquifers.
 288 We highlight that this study focuses on the heterogeneity of the hydraulic conductivity, thereby
 289 neglecting the variability of other parameters, such as thermal conductivity and capacity. This
 290 choice is justified by the fact that the hydraulic conductivity varies in much wider ranges and
 291 has a much stronger influence than both thermal conductivity and capacity. Piga et al. (2017)

292 highlighted that only the long-term (but not the short-term) propagation of thermal plumes is
 293 somehow affected by the thermal conductivity, whereas heat capacity has a negligible effect both
 294 in the short and the long term. When it comes to thermal feedback, much shorter time and space
 295 scales (i.e. the nearbies of the well doublet) are involved, compared to the propagation of thermal
 296 plumes (which develop over larger spatial scales compared to the well doublet distance). For
 297 this reason, even thermal conductivity has a secondary effect. Similar conclusions were achieved
 298 by Lo Russo et al. (2012).

299 We modelled the thermal plume by releasing $N_p = 5880$ particles from the injecting well.
 300 The injected mass is distributed around the injecting well at every $\pi/60$ radiant and placed
 301 uniformly along the depth with an offset of $2I_v$, which is needed in order to avoid boundary
 302 effect, from the top and the bottom of the domain. Figure 2 collects a few snapshots of the
 303 trajectories resulting from the application of the random walk particle tracking to our numerical
 304 system. The plane $x_1 - x_3$ is aligned with the regional flow and $\theta = 0$. The hydraulic conductivity
 305 field is generated with variance $\sigma_Y^2 = 2$. The figure shows as the particles placed in the highly-
 306 conductive layers travel faster (see dark orange layer in Figure 2). On the contrary, the particles
 307 in the low-conductive layers move very slowly (see light yellow layers in Figure 2).

308 Finally, flow and transport are performed on $MC = 500$ Monte Carlo realizations, which
 309 allow to obtain reliable estimates of the ensemble Breakthrough Curve (BTC). For each real-
 310 ization i , we collected the breakthrough time $\tau_{0,i}$ as the time needed for the fastest particle to
 311 reach the pumping well, and the recirculating ratio RR_i as the ratio between the number of
 312 particles at the pumping well to the total particles. The ensemble breakthrough time $\langle \tau_0 \rangle$ and
 313 recirculating ratio $\langle RR \rangle$ are then calculated as

$$\langle \tau_0 \rangle = MC^{-1} \sum_{i=1}^{MC} \tau_{0,i} \quad (14)$$

$$\langle RR \rangle = MC^{-1} \sum_{i=1}^{MC} RR_i \quad (15)$$

314 Assuming ergodic transport, the breakthrough curve at the pumping well is calculated as
 315 the Cumulative Distribution Function (CDF) of the travel times to the well considering all
 316 simulations together. The BTC is subsequently scaled with the initial local velocity in order
 317 to consider flux-proportional injection (see, e.g., Janković and Fiori, 2010; Pedretti and Fiori,
 318 2013; Fiori et al., 2017; Di Dato et al., 2017). The temperature at the production well is finally

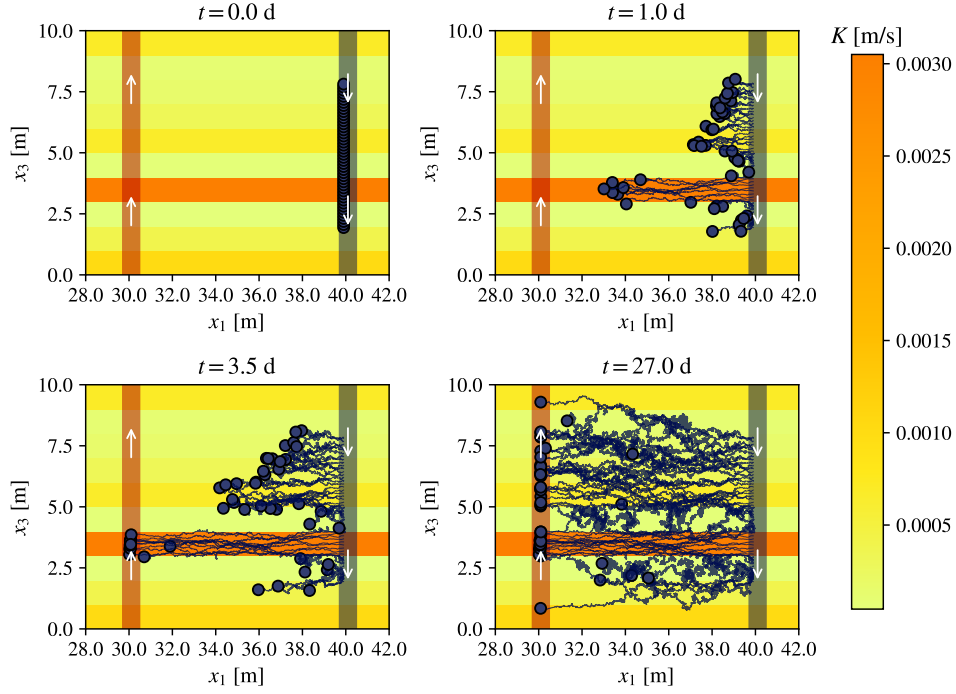


Figure 2: Four snapshots depicting the particle trajectories as a function of time. The plane $x_1 - x_3$ is placed at $x_2 = 0$. The two wells are aligned with the regional flow (i.e. $\theta = 0$). The thermal plume travels in a stratified medium with variance $\sigma_Y^2 = 2$, thermal diffusion $D_{th} = 10^{-6} \text{m/s}^2$ and thermal dispersivity $\alpha_d = 0.001 \text{ m}$.

319 calculated by counting the number of particles converging at the production well, as follows
 320 (Ferguson, 2006):

$$T_{prod}(t) = \frac{n(t)T_{well} + [N_p - n(t)]T_{ref}}{N_p} \quad (16)$$

321 where $n(t)$ is the number of particles that have been collected at the time t . The numerical code
 322 has been tested in order to verify that the number of Monte Carlo simulations and the number
 323 of injected particles are enough to reach statistical convergence.

324 The parameters used for the simulations and listed in Table 1 were chosen as representative of
 325 the geothermal systems typically designed (Galgaro and Cultrera, 2013; Piga et al., 2017). The
 326 scenarios comprise two values of hydraulic gradient J , two values for the effective conductivity
 327 K_{eff} , three values of angle θ , three values of heterogeneity degree σ_Y^2 , two values of α_d and D_{th}
 328 and thirteen pumping rates Q_w , for a total of 936 different combinations. In order to keep this
 329 number small, we fixed those parameters that impact only the temporal scale at which thermal

330 feedback occurs, such as the porosity n , the aquifer depth B , the distance between the wells
331 L , the thermal retardation factor R_{th} and the temperature difference between the two wells.
332 Generally the introduction of additional variability in the parameters involves an increase of
333 heterogeneity in the results. The findings obtained here could be enhanced by considering, for
334 instance, an heterogeneous porosity or a heterogeneous thermal dispersivity.

Parameter	Description	Value
Fixed parameters		
n	Porosity	0.1
B	Aquifer depth	10 m
L	Distance between the wells	10 m
R_{th}	Thermal retardation factor	3.4 ^a
I_v	Vertical integral scale	0.5 m ^b
T_{well}	Temperature at the injecting well	5°C
T_{ref}	Temperature in groundwater	15°C
Scenarios parameters		
θ	Angle between wells and regional flow	0, $\pi/4$, $\pi/2$
α_d	Pore-scale dispersivity	0, 0.001 m ^c
D_{th}	Thermal diffusion	0, 1e-6 m/s ² ^d
K_{eff}	Effective conductivity	0.001, 1e-5 m/s ^b
σ_Y^2	Variance of the log-conductivity field	Homog., 1, 2 ^b
J	Hydraulic gradient	0.01, 0.001
Q_w	Pumping rate	$X = [2 - 12]$ ^e

^a See Casasso and Sethi (2015); ^b See Rubin (2003, Table 2.2); ^c See Fiori and Dagan (1999); ^d
See Holman (2008, Appendix A, Table A-3); ^e The pumping rate is set up in order to obtain a
 χ varying between 2 and 12

Table 1: Model parameters for the numerical experiments.

335 3. Results and Discussion

336 Results are shown in terms of breakthrough time τ_0 , recirculating ratio RR and temperature
337 at the pumping well T_{prod} for different scenarios. We will analyze separately the impact of
338 pore-scale processes and the angle between the wells and the regional flow. In the first case,
339 the geothermal system is aligned with the groundwater flow (i.e. $\theta = 0$). In the latter case the
340 analysis is carried under pure advection (i.e. $\alpha_d = 0$ and $D_{th} = 0$).

341 3.1. Breakthrough time

342 The first analysis we introduce deals with the homogeneous domain. Figure 3 shows the
343 ratio τ_0/τ_{reg} as a function of χ , which represents the dimensionless pumping rate. Results are
344 normalized by $\tau_{reg} = KJ/(R_{th}nL)$, i.e. the time needed to travel the distance L when only
345 regional flow is considered.

346 In Figure 3a different markers pertain to different couples of (K, J) , which determine different
347 flow velocities in the system, whereas different colors are associated to different values of the pore-
348 scale processes α_d and D_{th} . Results show that generally τ_0/τ_{reg} decreases with an exponential
349 behaviour with χ , namely the higher the pumping rate, the shorter the first travel time. Such a
350 result is consistent with previous studies (Milnes and Perrochet, 2013; Casasso and Sethi, 2015).
351 Despite the general behaviour is similar, significant deviations from the purely advective solution
352 can be noticed in the cases with lower velocities. In fact, when advective velocity decreases, the
353 relative importance of diffusion increases. In such a case, the impact of thermal diffusion is
354 not negligible, while the effect of pore-scale dispersivity appears to be always irrelevant in any
355 simulated scenario. The previous analysis is supported by Figure 3b, which depicts a snapshot
356 of the particle trajectories for the considered scenarios with $D_{th} = 10^{-6}$ m/s². We highlight
357 that $D_{th} = 10^{-6}$ m/s² is the typical thermal diffusion among the values encountered in natural
358 aquifers (Holman, 2008). Inspection of figure shows that when the flow velocity is smaller
359 (scenarios 3 and 4), the dispersion processes prevail and the trajectories assume a more chaotic
360 pattern with respect to the scenarios where the advection prevails (1 and 2). As a consequence,
361 analytical solutions for the geothermal system design should be carefully taken into account even
362 for homogeneous media. In fact, by considering only advection, the analytical eq. (2) might
363 lead to a significant overestimation of the breakthrough time.

364 The application range of solution τ_0^{an} is explored in Figure 4, where the relative difference in

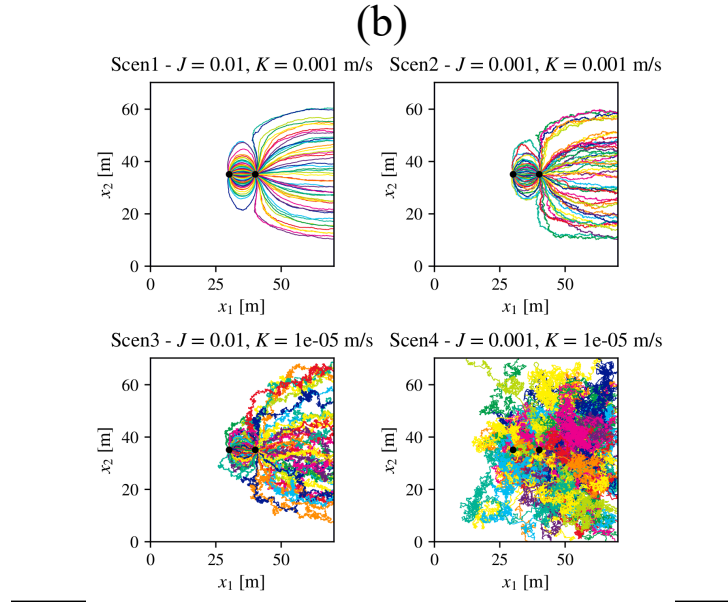
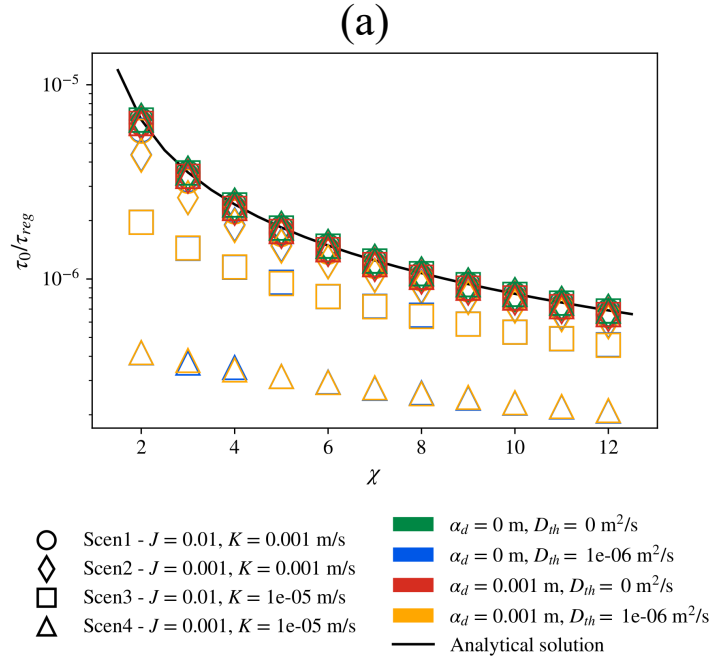


Figure 3: a) Normalized thermal breakthrough times τ_0/τ_{reg} as a function of the dimensionless pumping rate χ for several scenarios depicting different regional flow, i.e. combinations of K and J in a homogeneous medium. Results are normalized by the time a particle needs to cover the distance L under uniform flow and advective transport. b) Pathlines in homogeneous porous media as a result of different combinations of average gradient (J) and hydraulic conductivity values (K) of the porous medium when thermal diffusion is $D_{th} = 10^{-6}$ m/s².

365 predicted breakthrough time $|\tau_0 - \tau_0^{an}|/\tau_0^{an}$ is represented as function of D_{th} and χ . This ratio,
366 namely the normalized absolute error of the analytical solution, approaches the zero value when
367 advection is dominant, while on the opposite case, i.e. when it approaches the value of one,
368 pore-scale heat transport mechanisms play the key role. Scenarios 1 and 2 are characterized by
369 higher flow velocities and are associated with small errors, therefore the analytical solution can
370 be used and the effect of dispersion is negligible. Focusing on the fourth scenario, it is possible
371 to observe how the accuracy of the travel time assessed with eq. (2) decreases with decreasing χ ,
372 when the pumping rate is lower. In short, figure 4 confirms that the impact of heat conduction
373 on the breakthrough time is relevant only for low velocity systems, while advective transport
374 prevails in most cases.

375 We discuss now the effect of the heterogeneity of the hydraulic conductivity K on the break-
376 through time τ_0 . The medium heterogeneity, defined by the variance of the log-conductivity σ_Y^2 ,
377 has been recognized as a key parameter in transport problem in natural aquifers, since velocity
378 gradients due to K variability triggers macrodispersion phenomena (Matheron and De Marsily,
379 1980; Dagan, 1986; De Barros and Rubin, 2011; Zech et al., 2015; Di Dato et al., 2016). In this
380 study we consider two heterogeneity scenarios, depicted by formation with mild heterogeneity
381 degrees, i.e. $\sigma_Y^2 = 1$ and 2. Results are shown as a function of the dimensionless pumping rate
382 χ , which is defined by eq. (13) for the heterogeneous medium. The other parameters governing
383 the regional flow are kept constant and pertain to the second scenario in the previous paragraph,
384 i.e. $J = 0.001$ and $K_{eff} = 0.001$ m/s. It is worth noticing that in stratified media the effective
385 hydraulic conductivity corresponds to the arithmetic mean of K .

386 As in the previous paragraph, we analyze the mean breakthrough time $\langle\tau_0\rangle$, defined as the
387 expected value of the sample of the breakthrough times. The sample is composed of a number
388 of Monte Carlo simulations, i.e. $MC = 500$. The mean breakthrough time $\langle\tau_0\rangle$ is depicted as
389 a function of χ for four combinations of pore-scale dispersivity α_d and thermal diffusion D_{th} ,
390 as shown in Figure 5. The homogeneous solutions and the analytical function (see eq. (14))
391 are depicted too as reference. Generally the behaviour appears to be similar to the previous
392 analysis, with $\langle\tau_0\rangle$ that decreases for increasing χ values. As expected, the effect of the medium
393 heterogeneity is to reduce the $\langle\tau_0\rangle$, which decreases moving from the homogeneous case to the
394 $\sigma_Y^2 = 1$ and $\sigma_Y^2 = 2$ cases. Such behavior is a consequence of the larger sampling of the higher
395 values of the hydraulic conductivity involved by the higher σ_Y^2 . The higher values of K are

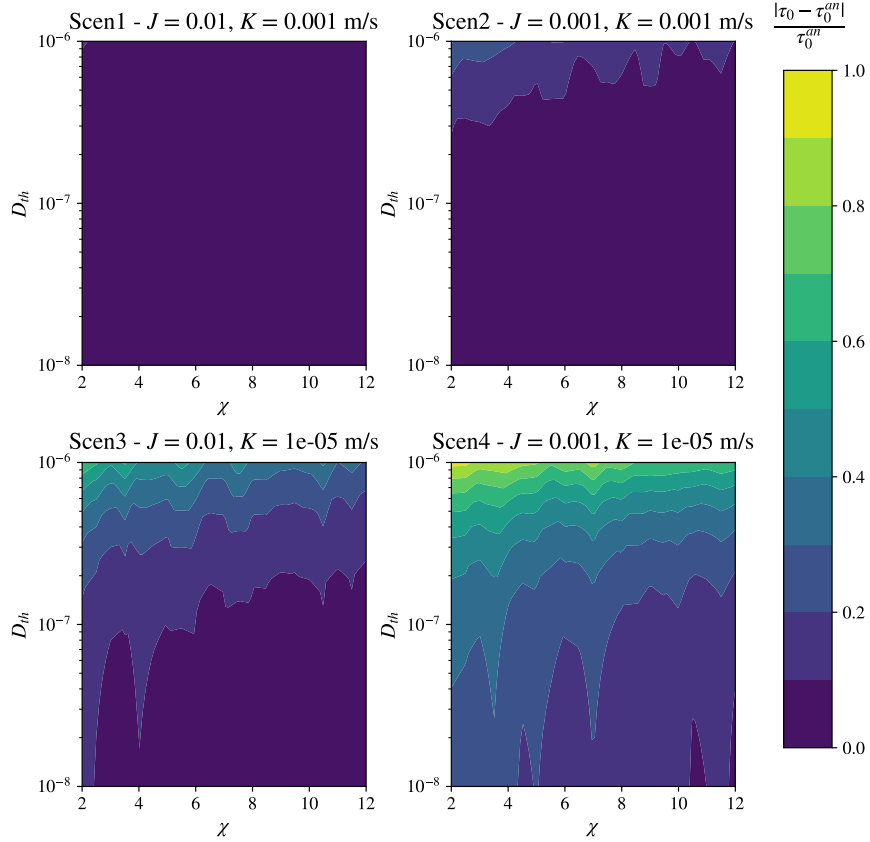


Figure 4: Contour plot of the difference between the numerical τ_0 and the analytical τ_0^{an} (eq. (2)) for χ and D_m and several regional flow scenarios. The plot provides also an indication of the governing transport mechanism, which is advective when $|\tau_0 - \tau_0^{an}|/\tau_0^{an}$ tends to zero and dispersive when $|\tau_0 - \tau_0^{an}|/\tau_0^{an}$ increases.

396 representative of the fast flow channels which develop in heterogeneous natural formations. As
 397 showed in Figure 2, the particles placed in the higher-conductivity layer travel much faster than
 398 the other ones. The inset of Figure 5 depicts also the coefficient of variation CV of τ_0 with
 399 respect to the MC realizations as a function of χ for several heterogeneity values. For the case
 400 $\sigma_Y^2 = 2$, CV shows values higher than 2. This result is of paramount importance because it
 401 indicates that τ_0 cannot be considered as a comprehensive index without the assessment of its
 402 variability.

403 When analyzing different geometrical configurations obtained by varying the angle θ between

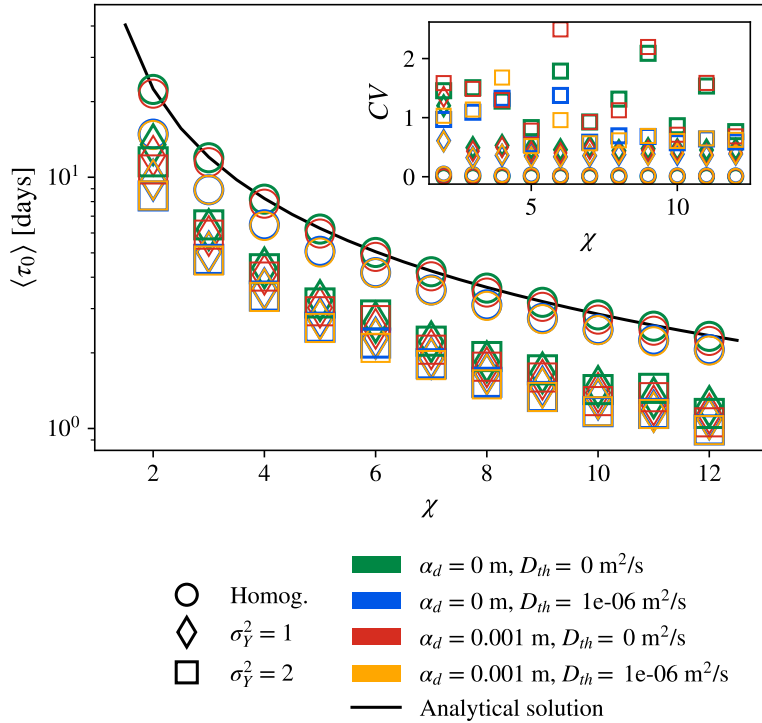


Figure 5: Mean breakthrough time $\langle \tau_0 \rangle$ [d] as a function of χ for several values of hydrodynamic dispersion α_d and thermal diffusion D_{th} . The inset depicts the coefficient of variation CV . The mean value and the CV are calculated over a sample of $MC = 500$ Monte Carlo simulations. Results are calculated for a well doublet aligned to the regional flow (i.e. $\theta = 0$).

404 the wells and the regional flow, the most efficient setup is for θ equal to zero. Otherwise, by
 405 increasing the angle between the wells and the regional flow, the breakthrough time decreases,
 406 as shown in Figure 6. This result is consistent with previous studies (Milnes and Perrochet,
 407 2013; Casasso and Sethi, 2015). Such an aspect should be taken into consideration in practical
 408 application, given that groundwater direction might be affected by seasonal variation (Bellin
 409 et al., 1996).

410 It should be highlighted that in both cases, the results show slight differences in the mean
 411 $\langle \tau_0 \rangle$ when σ_Y^2 changes from 1 to 2. Liu et al. (2019) performed a similar analysis by studying the
 412 relationship between thermal breakthrough time and conductivity heterogeneity with a variance
 413 ranging between 0 and 6. As in the present work, they observed that the breakthrough time
 414 decreases non-linearly with σ_Y^2 , with smaller differences in the higher heterogeneity cases. In
 415 contrast, the uncertainty associated to τ_0 in a single realization increases dramatically with

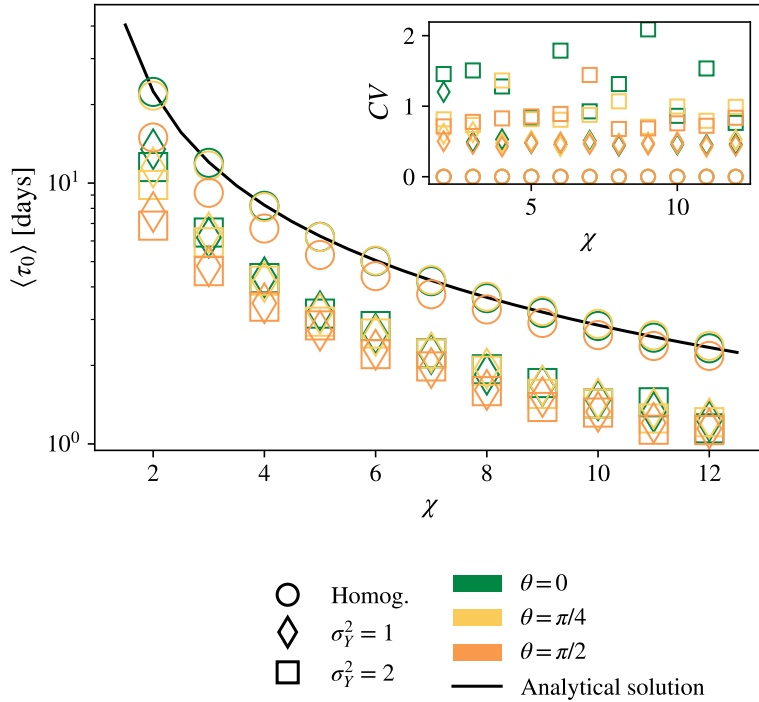


Figure 6: Mean breakthrough time $\langle \tau_0 \rangle$ [d] as a function of χ for several values of the angle between regional flow and wells θ . The inset depicts the coefficient of variation CV . The mean value and the CV are calculated over a sample of $MC = 500$ Monte Carlo simulations. Results are calculated under advection-only transport (i.e. $\alpha_d = D_{th} = 0$).

416 heterogeneity, as shown by the coefficient of variation CV in the insets of both Figures 5 and 6.
 417 However, such an uncertainty decreases with the number of layers when ergodicity is reached.
 418 Such an issue will be discussed later in a dedicated paragraph.

419 3.2. Recirculating ratio RR

420 Along with the breakthrough time, which is an indicator of the early arrivals, the other
 421 main operational metric of open-loop geothermal well doublets is the recirculating ratio RR ,
 422 i.e. the fraction of the flow returning from the injection well to the production well, which is
 423 instead an indicator of the long-term effects of returning flow. Figure 7 depicts the effect of
 424 pore-scale dispersivity and thermal dispersion for both homogeneous and heterogeneous media
 425 on the mean recirculating flow $\langle RR \rangle$. The results show that conductivity heterogeneity as well
 426 as thermal dispersion processes generally have a small impact on $\langle RR \rangle$, significant differences
 427 can be noticed only for the lower normalized pumping rate $\chi < 6$. Low pumping rate magnifies

428 the effect of preferential paths, thereby increasing the probability of particles to come back to
 429 the production well. The coefficient of variation of $\langle RR \rangle$, shown in the inset, increases with σ_Y^2
 430 and decreases with χ pointing at an higher uncertainty in domains characterized by an high
 431 heterogeneity degree and a lower pumping rate.

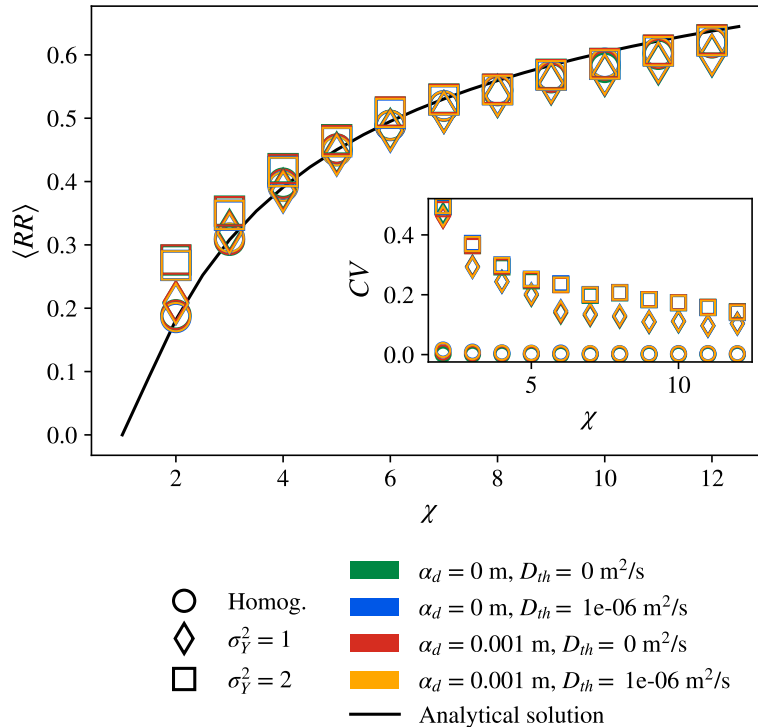


Figure 7: Mean recirculating ratio $\langle RR \rangle$ as a function of χ for several values of hydrodynamic dispersion α_d and thermal diffusion D_{th} . The inset depicts the coefficient of variation CV . The mean value and the CV are calculated over a sample of $MC = 500$ Monte Carlo simulations. Results are calculated for a well doublet aligned to the regional flow (i.e. $\theta = 0$).

432 Figure 8 shows the mean recirculating ratio $\langle RR \rangle$ as a function of χ for several values of
 433 θ , for both homogeneous and heterogeneous media under only advection (i.e. $\alpha_d = D_{th} = 0$).
 434 The most efficient configuration is when the wells and the regional flow are aligned, following
 435 the breakthrough time behaviour. As in the previous analysis, when χ is large the effect of the
 436 heterogeneity is negligible on both the average value of $\langle RR \rangle$ and its variation coefficient.

437 Furthermore we notice that while the CV for the τ_0 was around one, the CV for RR is smaller
 438 than 0.2 for large χ . Such a result indicates that the uncertainty related to the recirculating
 439 volume is less affected by heterogeneity than breakthrough time. From a practical point of

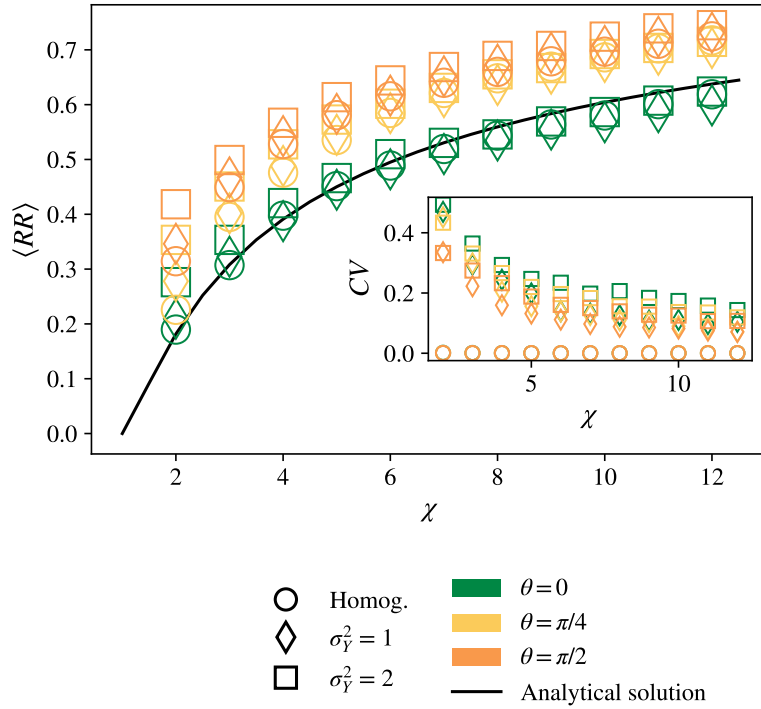


Figure 8: Mean recirculating ratio $\langle RR \rangle$ as a function of χ for several values of the angle between regional flow and wells θ . The inset depicts the coefficient of variation CV . The mean value and the CV are calculated over a sample of $MC = 500$ Monte Carlo simulations. Results are calculated under advection-only transport (i.e. $\alpha_d = D_{th} = 0$).

440 view, this implies that the recirculating flow rate can be determined by considering the effective
 441 conductivity instead of homogeneous conductivity. Consequently, the results from the analytical
 442 solution can be a robust evaluation tool.

443 3.3. Temperature at the pumping well

444 Evaluating breakthrough times is key to assess whether thermal feedback will occur. Indeed,
 445 even if $\chi > 1$, the breakthrough time is often larger than the duration of the heating/cooling
 446 season and, hence, the water temperature at the production well remains unaltered. However,
 447 the efficiency of the system does not depend on whether thermal breakthrough time occurs or not,
 448 but on the time trend of operating temperatures. This holds true *a fortiori* for heterogeneous
 449 aquifers, where thermal breakthrough time may occur within a very short time. As depicted by
 450 the snapshots in Figure 2, the heterogeneous field is composed of alternating layers of high and
 451 low conductivity. Consequently, particles in the high-conductive layers reach the production

452 well earlier than particles in the other zones. In contrast, the particles trapped in the low-
 453 conductivity zones extend the arrival time of the last part of the plume. Therefore considering
 454 τ_0 only would mislead the evaluation of the operational sustainability of the system. For this
 455 reason, we also analyzed the long-term evolution of water temperatures at the production well.
 456 Figure 9 shows the temperature time trends for several typical values of χ and for four
 457 combinations of hydrodynamic dispersion α_d and thermal diffusion D_{th} . Figure 10 depicts the
 458 temperature evolution as a function of heterogeneity for several values of θ .

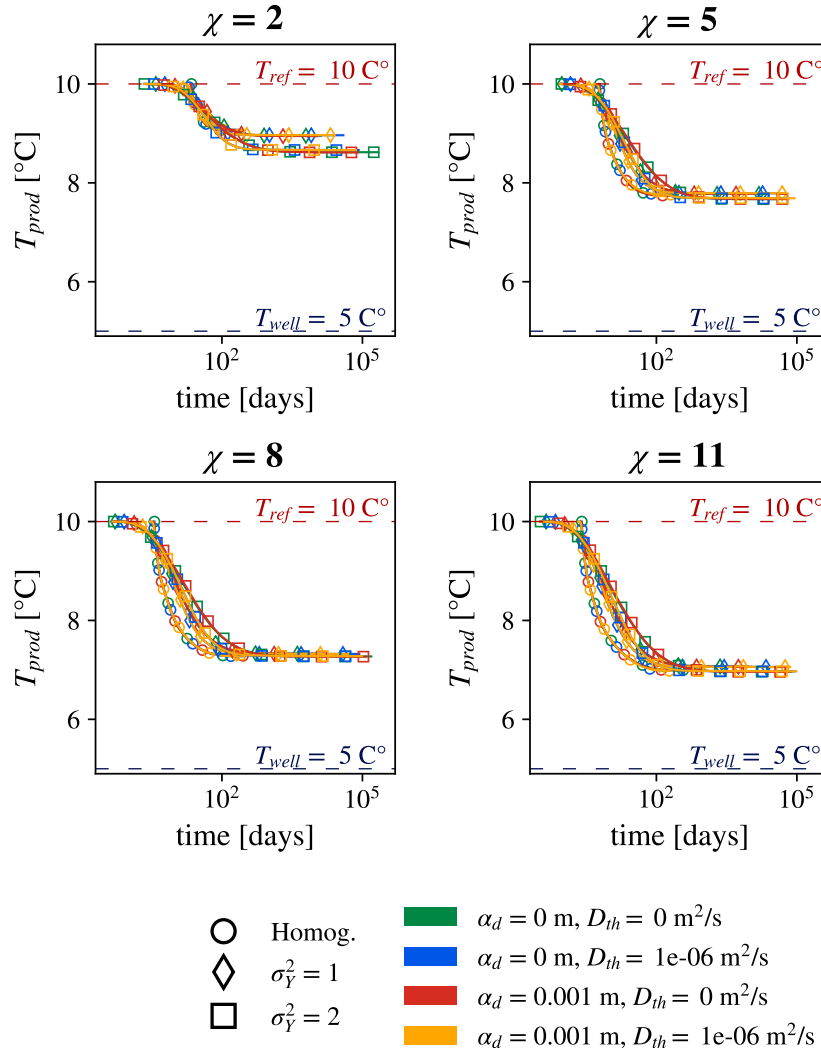


Figure 9: Temperature at the pumping well for several χ values and for four combinations of hydrodynamic dispersion α_d and thermal diffusion D_{th} . Results are calculated for a well doublet aligned to the regional flow (i.e. $\theta = 0$).

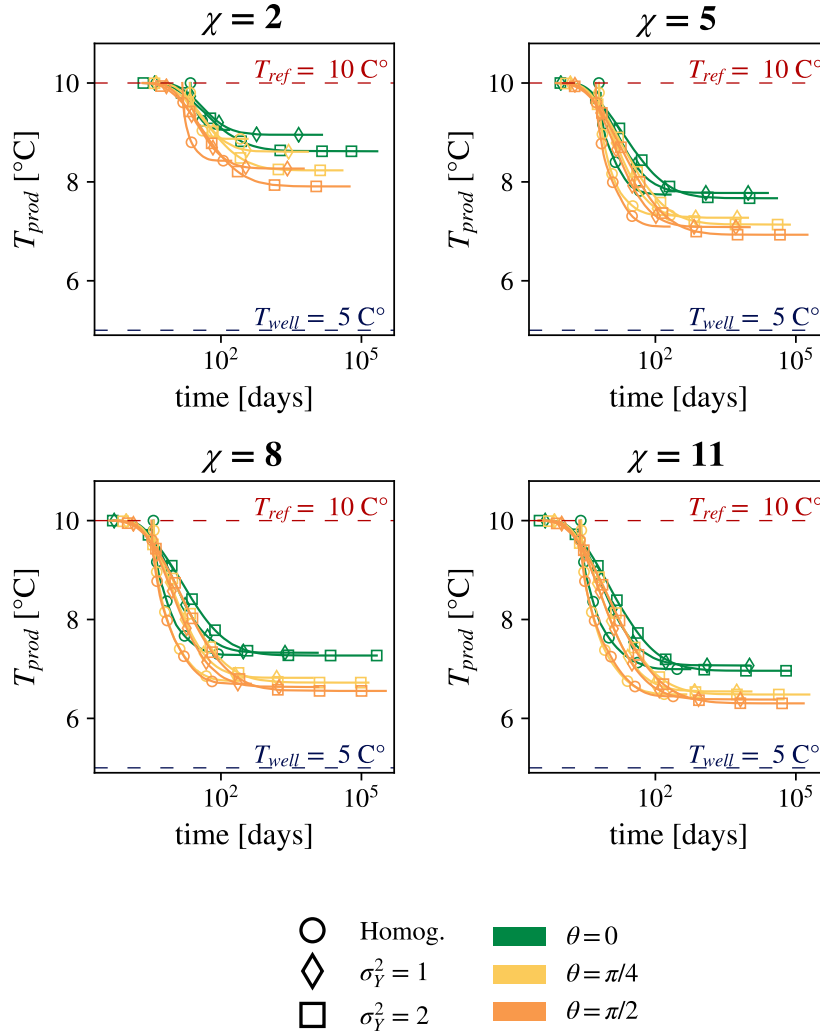


Figure 10: Temperature at the pumping well for several χ values and for several values of θ . Results are calculated under advection-only transport (i.e. $\alpha_d = D_{th} = 0$).

459 Both figures confirm that the plume dispersion at the production well increases with heterogene-
 460 ity, in line with experimental evidences (Sauty et al., 1982; Park et al., 2018). Heterogeneity
 461 has a strong influence on the breakthrough time and on the shape of thermal breakthrough
 462 curve. Also Babaei and Nick (2019) observed a similar behavior. Their study shows that con-
 463 ductivity heterogeneity reduces the time needed to drop the temperature by 1°C when the initial
 464 temperature is of 75°C and the reinjection is at 30°C .

465 In contrast, conductivity heterogeneity is negligible for the long-term development of ther-
 466 mal feedback, as already observed for the recirculating ratio RR . Such behavior becomes more

467 evident by increasing χ , when advection dominates over heat conduction. Although the break-
468 through time decreases with heterogeneity, the overall efficiency of the system benefits from it.
469 In fact, the temperature decreases faster when the medium is homogeneous, as shown by the
470 lines with circle markers in Figures 9 and 10. The effect of thermal dispersion on BTC shape
471 increases with medium heterogeneity: while the four BTCs overlap for homogeneous medium,
472 heterogeneity causes a departure in BTCs depending on the D_{th} value. Thermal diffusion ac-
473 celerates the development of thermal feedback as well, as shown in Figure 9.

474 The angle θ has a small impact on the thermal breakthrough time, for which the effect of
475 heterogeneity predominates. In contrast, the BTC long-term behavior is controlled mainly by
476 the well doublet angle θ and heterogeneity plays a negligible effect.

477 3.4. The ergodicity issue

478 As stated previously, the *CV* in the insets of Figures 5-8 shows the uncertainty associated
479 to heterogeneity. In the present study, the coefficient of variation indicates the dispersion of the
480 single realizations around their ensemble mean. Here we have considered a sample of $MC =$
481 500 Monte Carlo realizations. However, the coefficient of variation decreases by increasing the
482 aquifer depth. When the wells are deep enough to totally grasp the variability of conductivity
483 heterogeneity, the single realization approaches the ensemble mean. Only under such a case, it
484 is possible to assume the ergodic condition, which allows to consider the single realization as
485 representative of the ensemble mean (Kitanidis, 1988; Dagan, 1991; Fiori, 1998; Dentz et al.,
486 2000). Given that well screens usually cross a short depth (typically from a few meters to a
487 few tens of meters), ergodicity could not always be assumed, thereby increasing the uncertainty
488 associated with the predicted ergodic BTC. Figure 11 shows the BTCs for each realization and
489 the ensemble BTCs averaged over an increasing number of Monte Carlo simulations (MC).

490 For the case considered here, i.e. aquifer depth is composed of ten layers, the single BTC
491 realization can significantly differ from its ergodic counterpart. As a practical consequence,
492 a thermal feedback occurring in a heterogeneous medium could significantly differ from the
493 expected theoretical one, which typically assumes ergodicity. Moreover, the uncertainty of the
494 single realization increases with medium heterogeneity. Figure 11 shows that ergodic conditions
495 are reached averaging over 10 to 20 realizations, which correspond to 100-200 layers according to
496 the heterogeneity degree. As a consequence, the analysis associated to this kind of uncertainty
497 should be carefully considered while designing geothermal systems in heterogeneous media.

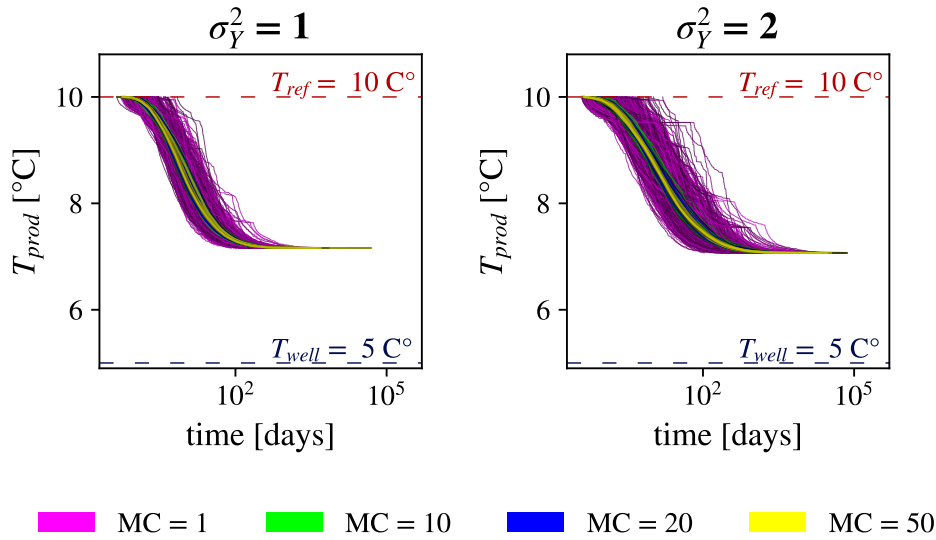


Figure 11: Sample of BTCs used ($MC = 500$ realizations) and the ensemble BTC as function of the MC simulations (layers).

498 This last issue is of paramount importance in studies dealing with the efficiency of geothermal
 499 systems. When the exploitation plant is made of wells crossing a small number of geological
 500 formations, the temperature evolution in time can significantly differ with the expected one,
 501 based on model results, whose parameters are usually defined by a limited number of tests. In
 502 contrast, modeling results are more reliable when the wells cross a large number of geological
 503 formations. Finally we highlight that additional sources of uncertainty on results could arise
 504 considering variability in other parameters, such as the porosity or the thermal dispersion, which
 505 are kept constant within this extensive analysis. Despite this we believe that our results can be
 506 considered as general and can provide a suitable basis for a more reliable efficiency assessment
 507 of shallow geothermal energy systems.

508 4. Conclusions

509 The present study analyzed the interplay of thermal dispersion and macrodispersion in heat
 510 transport, thereby focusing on the role of heterogeneity and thermal dispersivity in the design
 511 of open-loop shallow geothermal systems. We analyzed the following metrics: the breakthrough
 512 time, corresponding to the time the reinjected water needs to reach the production well; the
 513 recirculating rate, i.e. the fraction of injecting water returning to the production well; and the

514 temperature curve at the production well.

515 The main findings are:

- 516 • The effects of thermal dispersion parameters are strictly related to the pumping rates and,
517 in general, to the groundwater velocity values. In general, thermal dispersion becomes
518 appreciable in systems characterized by low pumping rates.

- 519 • The heterogeneity has a strong impact on the early operational time of geothermal well
520 doublets. Due to channeling, the thermal plume travels faster in the highly conductive
521 layers. As a result, the breakthrough time decreases with heterogeneity. Moreover, the
522 uncertainty associated with early arrivals increases with heterogeneity. Such behavior
523 confirms evidences already observed by Liu et al. (2019) and Babaei and Nick (2019).

- 524 • The heterogeneity, as well as dispersion and convection, has a negligible effect on the
525 long-term period. The recirculating ratio depends strongly on the parameter χ and the
526 angle θ , namely it can be modelled by assuming advection only. Therefore the analytical
527 solution for the recirculating ratio RR^{an} gives a robust assessment of the long-term system
528 sustainability.

- 529 • The thermal plume spreads more when increasing the variance of medium conductivity.
530 The breakthrough time can therefore be misleading as an indicator of the system efficiency
531 and the whole thermal BTC should be considered. Heterogeneity should be carefully con-
532 sidered, because trajectory dispersion magnifies the variance of arrival times. In highly
533 heterogeneous aquifers, the time span between thermal breakthrough time and a substan-
534 tial development of thermal feedback can be long enough for the heating/cooling season
535 to end. Consequently the system could benefit from the medium heterogeneity. On the
536 other hand, the uncertainty due to non-ergodic conditions should be taken into serious
537 consideration as well.

538 The present work can be considered as a first step towards a better understanding of the cou-
539 pled effect of aquifer heterogeneity and engineering design on the efficiency of shallow geothermal
540 systems. Despite significant assumptions were adopted (i.e. stratified formation, steady state
541 flow, constant injection temperature), the study highlighted and explained noteworthy mod-
542 elling issues. For instance, we found that heterogeneity has a minor impact on the long-term

543 behavior, but it has a tremendous impact on the short-term counterpart. As a consequence, the
544 assessment of the system efficiency should rely not only on the breakthrough time, but also on
545 the complete temperature evolution at the production well. In contrast, simplified analytical
546 solutions assuming only advection work well to assess the long-term sustainability of the system.

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