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Innovative numerical procedure for simulating Borehole Heat Exchangers operation and interpreting Thermal Response Test through MODFLOW-USG code

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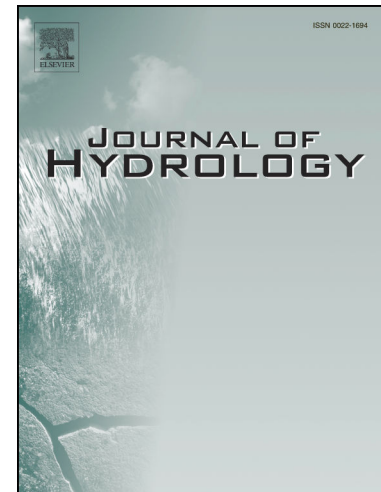
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1 **Innovative numerical procedure for simulating Borehole Heat Exchangers operation and interpreting**
2 **Thermal Response Test through MODFLOW-USG code**

3

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10 **Abstract**

11 In recent years, among renewable energies, the geothermal resource exploitation shows a constant growth;
12 specifically, in countries engaged in CO₂ emissions reduction and dependent on energy from abroad, the low-
13 temperature geothermal energy (geo-exchange) for air conditioning of buildings represents a cost-effective
14 and green solution. In closed-loop systems borehole heat exchangers (BHE) are coupled with ground-source
15 heat pumps (GSHP) constituting the key component of the heating ventilation air-conditioning (HVAC)
16 system. Therefore, the design of the BHE and the correct interpretation of in situ Thermal Response Tests
17 (TRT) are essential to supply the building energy demand. To support the design, Modflow-USG Connected
18 Linear Network (CLN) and Drain Return Flow (DRT) packages are adapted and improved to reproduce the
19 operation of one or more BHE in aquifers and to analyze the TRT. The improvements are compared with a
20 previously developed numerical model and two different analytical solutions (infinite line source and moving
21 line source) by imposing a constant heat rate injection into the aquifer. The results show good agreement
22 between the new approach and previous ones (discrepancy lower than 2% for models with highly refined
23 grid), but the new approach is much more accurate and expeditious in both implementation and execution,
24 also allowing for an easy numerical simulation of multiple BHE.

25

26 **Highlights**

- 27 - Improvement of CLN and DRT packages of MODFLOW-USG for BHE numerical simulation
- 28 - Testing of new procedure against previous numerical model and analytical solution
- 29 - Possibility to reproduce typical GSHP system and Thermal Response Test operation
- 30 - Easy and expeditious implementation of large borefield in a numerical model

31

32 Keywords

33 Heat transport modeling; MODFLOW-USG; Borehole Heat Exchanger; Ground-Source Heat Pump; Thermal
34 Response Test

35 1. Introduction

36 EU legislation evolved significantly to achieve the EU Paris Agreement commitments for reducing greenhouse
37 gas emissions by setting, through EC 2018/2001 Directive, the share of renewable energy by 2030 equal to
38 32% of final energy consumption. As buildings are responsible for around 36% of energy consumption and
39 for 34% of CO₂ emissions in Europe (European Commission, 2021), in 2016 through the “Clean Energy for all
40 Europeans package” it was possible to target the efficiency improvement of new and existing buildings, by
41 requiring an annual increase in the heating and cooling use of renewables of about 1.3%.

42 Since Ground-Source Heat Pump (GSHP) and Groundwater Heat Pump (GWHP) systems are among the
43 cleanest and most energy efficient Heating Ventilation and Air-Conditioning (HVAC) systems for buildings,
44 the exploitation of this technology has been expanding all over the world in recent years (Chae et al., 2022;
45 Farabi-Asl et al., 2019; Jodeiri et al., 2022; Lyu et al., 2020; Sakellari, D.; Lundqvist, 2003). According to the
46 last pre-pandemic statistical report by GSE (Italian Energy Services Manager), in 2019 in Italy 3392 Terajoules
47 of thermal energy were produced by exploiting GSHP or GWHP systems: although it represents only 0.15%
48 of the total consumed thermal energy, it increases at a yearly rate of 1.5%.

49 GSHP systems are coupled to the ground by means of a closed-loop ground heat exchanger. The latter can
50 either be composed of vertical U-shape pipes (called Borehole Heat Exchangers, BHEs), or of horizontal pipes,
51 where a non-freezing fluid (water mixed to glycol solution) is circulated to absorb heat from the ground

52 during the cold season and inject it during the warm one (Lyu et al., 2020). On the other hand, GWHP systems
53 are based on injecting and extracting wells (open-loop system), similar to those generally used for
54 Pump&Treat systems (Antelmi et al., 2020b) except that in this case water is used to produce energy. The
55 Coefficient of Performance (COP) of these systems reaches higher values than conventional air-source heat
56 pumps, since the ground is often cooler in summer and warmer in winter than the air temperature (Li et al.,
57 2014).

58 GSHP systems performance and design is highly dependent on the heat transfer capability between the BHE
59 and the subsoil, and thus the estimate of the thermal subsoil properties is essential (Pambou et al., 2022).
60 The execution of the so-called Thermal Response Test (TRT) on subsoil is always recommended for a better
61 HVAC system design and sometimes it is also mandatory: e.g., in Lombardy Region, Italy, a TRT is required
62 (Regione Lombardia, 2010) for GSHP systems with heat rate greater than 50 kW. This test is performed to
63 evaluate the effective thermal conductivity of the soil λ_{eff} and the borehole thermal resistance R_b (Gehlin,
64 2002; Spitler and Gehlin, 2015; Zhang et al., 2014). It is carried out on a pilot BHE connected to a testing unit
65 and is performed by supplying a constant heat rate to the circulating fluid by means of an electrical resistance
66 (Naldi and Zanchini, 2019). Inlet and outlet fluid temperatures are recorded throughout the test along with
67 water flow rate, electrical power related to the thermal resistance and external air temperature. (Blasi and
68 Menichetti, 2012) stated that the standard deviation of the thermal conductivity is equal to $\pm 15\%$ when the
69 test is conducted with a duration of about 20 hours, whereas it is reduced to $\pm 5\%$ for a test lasting about 50
70 hours. The presence of groundwater flow could complicate the assessment of the thermal conductivity, so
71 that performing the test over 72 hours is suggested; indeed, over that time, the available literature suggests
72 that the ground response to the thermal excitation achieves a steady-state condition for all aquifers that
73 have been studied (Antelmi et al., 2021; Beier, 2021; Nieto et al., 2020; Zhang et al., 2022).

74 Different approaches can be applied to the analysis of the experimental data recorded during the TRT: both
75 simplified analytical models (Banks, 2012; Carslaw and Jaeger, 1959; Diao et al., 2004; Molina-Giraldo et al.,
76 2011; Pasquier and Lamarche, 2022) and more complex numerical models allowing to include more elements
77 that influence test results (Casasso et al., 2017; Casasso and Sethi, 2014; Zong et al., 2021). Due to their

78 simple mathematical formulation and to the limited number of input parameters, the analytical models of
79 the Infinite Line Source (ILS) and the Moving Line Source (MLS) are the most common approaches adopted
80 for the interpretation of TRT data (Carlslaw and Jaeger, 1959; Diao et al., 2004). Both models assume the
81 GSHP system as an infinite linear heat source exchanging heat with the homogeneous and isotropic
82 surrounding ground with a constant heat flux per unit length (Bandos et al., 2009; Eskilson, 1987; Man et al.,
83 2010; Zeng; et al., 2002). The difference between the two models is that the ILS assumes pure conduction in
84 the ground, whereas the MLS also considers the advection term due to groundwater flow. Therefore, the ILS
85 model application is restricted to the geological sites where groundwater flow is absent or negligible,
86 otherwise, a more suitable solution is the MLS (Diao et al., 2004; Sutton et al., 2003; Wagner et al., 2013). In
87 the end, applying both the ILS and MLS, only an effective value of the thermal conductivity for the entire
88 depth of the BHE is obtained, neglecting the variation along the vertical caused by a heterogeneous
89 lithostratigraphy.

90 Numerical models represent a more complex but potentially more precise solution to evaluate the correct
91 aquifer thermal parameters (Attard et al., 2020; Fujii et al., 2005; Giordano et al., 2021). They need more
92 input parameters derived from a specific Conceptual Site Model (CSM), but they are flexible tools able to
93 simulate non-ideal conditions (e.g., heterogeneous soils, realistic surface boundary conditions, geothermal
94 gradients etc.) and relevant physical processes (namely, beside conduction, advection and thermal
95 dispersion). These tools coupled with suitable parameter estimation procedures provide more accurate
96 results (Antelmi et al., 2020a; Dalla Santa et al., 2022; Galgaro et al., 2021). When reproducing a BHE in a
97 numerical model, the main components involved are characterized by different dimensions: from millimetres
98 (pipe thickness) to meters (aquifer) (Angelotti et al., 2014a). When a fully 3-D approach is applied, the
99 multiple spatial scales lead to numerical models affected by high computational loads. (Angelotti et al.,
100 2014b) developed a 3-D numerical finite-difference model by means of MODFLOW code coupled to MT3DMS
101 of a single BHE by turning its circular section to an equivalent square one. Although the numerical model was
102 validated for different groundwater flow velocities, its applicability was limited due to the large number of
103 model domain cells that did not allow to represent more than one BHE. (Marcotte and Pasquier, 2008),

104 simulating the thermal behaviour of a vertical BHE, implemented a 3-D finite element numerical model
105 through the COMSOL code; by exploiting the symmetry of the problem they were able to halve the number
106 of cells and partially reduce the computational burden.

107 The reduction of the cells number for aquifer and BHE representation was also achieved using a 1-D (Shonder
108 and Beck, 1999) and a 2-D numerical modelling approach (Berberich et al., 1994; Wagner and Clauser, 2005)
109 or alternatively, by applying a reduced-order numerical approach that couples a 1-D description of the
110 vertical pipes heat transfer with a 3-D description of the aquifer (Signorelli et al., 2007). The latter created a
111 finite-element model of a BHE system in the fractured geological formation, which is suitable to simulate
112 coupled hydraulic and thermal processes under non-steady conditions. The authors used synthetic TRT data
113 from the numerical model to evaluate the sensitivity of the ILS model analysis to test duration, borehole
114 length, groundwater velocity and subsurface heterogeneity. The model implemented 3-D elements
115 reproducing the porous matrix around the BHE and 1-D pipe elements for the BHE implementation; the heat
116 transfer between the circulating fluid and the aquifer was simulated as a thermal resistance related to the
117 velocity-dependent heat transfer coefficient of the fluid. A similar method is used also in (Lamarche et al.,
118 2010) to compare different empirical and theoretical approaches for the evaluation of the borehole
119 resistance. The authors implemented a 3-D numerical model in COMSOL reproducing the borehole by means
120 of 1-D finite elements using the traditional advective equation. Another study developed in COMSOL is the
121 one by (Bozzoli et al., 2011), where a Two-Step Parameter Estimation Procedure (TSPEP) for the evaluation
122 of the grout and soil thermal conductivities is validated using both simulated and experimental data. As for
123 the previous studies, heat transport in the BHE was simulated through 1-D equations, while heat transfer in
124 the hydrogeological domain through 3-D equations. (Brunetti et al., 2017; Šimůnek et al., 2016) adopted the
125 coupling of a 2-D domain to implement the aquifer and a 1-D domain for the BHE in the HYDRUS code. The
126 two domains were connected by a Robin boundary condition which enabled the simulation of heat transfer
127 between the BHE and the surrounding soil. The proposed numerical TRT was validated against experimental
128 data collected in two sites in Japan. Similar studies about pseudo-3-D models for the simulation of GSHP
129 operation are reported in (Al-Khoury et al., 2005; Florides et al., 2012; Raymond et al., 2011).

130 The aim of the present study is to provide an updated, simple, improved and expeditious numerical tool to
131 analyse in situ TRT through MODFLOW, specifically the version MODFLOW-USG, a widely used code for
132 modelling environmental problems in groundwater. The novelty of the updated tool is the introduction into
133 the CLN package of new characteristic elements of a BHE, such as the thickness and the thermal conductivity
134 of the U-pipe and the internal convective heat transfer coefficient. Another important improvement is the
135 option to couple the Connected Linear Network (CLN) and Drain Return Flow (DRT) packages, to simulate the
136 heat carrier fluid circulating in the BHE and injecting a constant heat rate into the ground. This allows to
137 simulate a TRT and to validate the CLN approach comparing it with the available constant heat rate analytical
138 solutions. These enhancements are key to reproduce each thermal resistance between the circulating fluid
139 and the aquifer, thus accurately reproducing the heat transfer nearby the BHE through a 1-D approach for
140 the fluid. Therefore, besides providing an effective method to simulate and analyse a TRT, the proposed tool,
141 without the DRT Package, can be used to expeditiously simulate the typical operation (heating/cooling) of a
142 GSHP system consisting of multiple BHE avoiding numerical convergence problems. In the present paper
143 different numerical models at constant heat rate injection are developed, featuring four spatial
144 discretizations, and a sensitivity analysis on groundwater velocity is performed. Each model is then tested
145 against common analytical models (ILS and MLS) and compared with the numerical models discussed in
146 (Angelotti et al., 2014a).

147 2. Material and methods

148 A synthetic numerical model of a single BHE with hydrogeological and thermal properties adapted from
149 (Angelotti et al., 2014a), is implemented in MODFLOW-USG by applying the approach tested in (Antelmi et
150 al., 2021). The graphical user interface is Groundwater Vista 7.0 (ESI, Inc.). The CLN package has been
151 updated in some programming features compared to the version package discussed in (Antelmi et al., 2021);
152 whereas, the DRT package is specifically adapted to create a constant heat rate injection in aquifer, such as
153 in TRT execution. A complete description of the package modification is presented in the next pages.

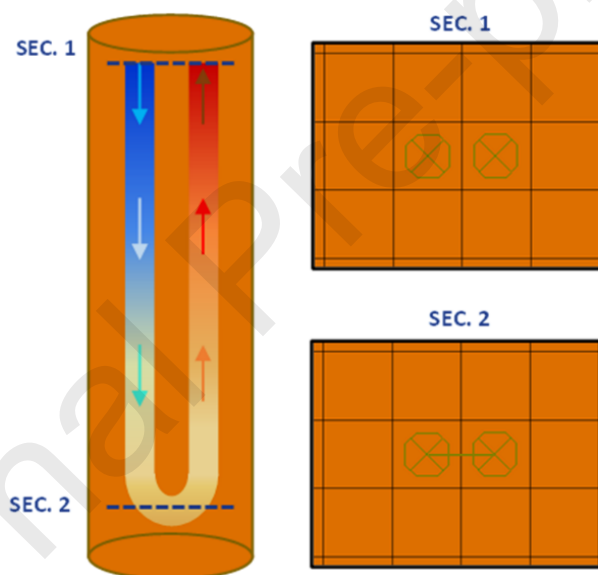
154 2.1 MODFLOW-USG and CLN

155 MODFLOW-USG (Panday et al., 2013) is an open access numerical code for modeling groundwater flow. The
156 main advantage over previous versions of MODFLOW is the Control Volume Finite Difference (CVFD)
157 approach, which is a generalization of the finite-difference approach that allows the use of unstructured
158 grids. The other characteristic that distinguishes MODFLOW-USG is the solution of tightly coupled processes
159 that interact with groundwater flow; thus, every equation of the model is solved in one matrix, avoiding
160 convergence problems. Specifically, the CLN package simulates one-dimensional features such as pipes,
161 wells, karst conduits, or streams that interact with groundwater flow. Since its release, MODFLOW-USG has
162 been expanded to include solute and heat transport; such features are available as open access software
163 USG-Transport (Panday, 2020). The Heat Transport Package is well suited for simulating geothermal plants
164 impacts and CLN Package is well suited to simulate a BHE, as it was demonstrated by (Antelmi et al., 2021).
165 In previous works, the numerical modeling of BHE with MODFLOW/MT3DMS was faced for the first time by
166 (Angelotti et al., 2014a). That paper aimed to prove the capability of these codes to model BHEs with a good
167 accuracy and to fully discuss the influence of groundwater flow on the energy performance of BHEs and on
168 the aquifer temperature distribution. The U-pipe geometry, the thermal-carrier fluid flow and aquifer
169 temperature distribution were explicitly reproduced for the first time, going beyond previous applications of
170 numerical codes. The main challenge was to correctly reproduce the BHE in a homogeneous aquifer through
171 a square or rectangular grid (classic Finite Difference grid of MODFLOW-2000). To this purpose, the U-shape
172 pipe was represented by a square section requiring a very fine horizontal and vertical discretization
173 (minimum cell size 0.37 cm). The pipe size was derived on the assumption of conserving the total thermal
174 resistance per unit length between circular section and square one. In specific, the total thermal resistance
175 was calculated as the sum of a convective resistance and of a conductive one.

176 An extensive validation of the numerical model solutions was provided comparing them with the analytical
177 MLS solution, assimilating the U-pipe to an infinite line source and varying the groundwater velocity. The
178 heat exchange rate was not imposed as a boundary condition but resulted from the interaction between the
179 BHE and the surrounding porous medium. The simulation results provided an evaluation of the temperature

180 perturbation in the aquifer, improving the energy exchange estimation and providing a quantitative
 181 assessment of the heat rate increase due to groundwater flow.

182 CLN elements can be vertical, horizontal, or inclined and can have rectangular or circular shaped cross-
 183 sectional geometries. Their connection for flow and transport to groundwater flow (GWF) cells occurs
 184 through analytic equations that include skin/efficiency factor considerations. MODFLOW-USG
 185 accommodates vertical, horizontal, or angled CLN elements. Groundwater Vistas allows for input of CLN as a
 186 "CLN well" or a "CLN polyline": the former is vertical and used to represent vertical conduits (e.g., a well),
 187 while CLN polylines can be implemented at any angle (e.g., hydraulic pipes). In the current implementation,
 188 the CLN polyline is used to connect 2 vertical CLN wells to reproduce the real geometry (U-shape pipe) of the
 189 BHE (Figure 1).



190

191 *Figure 1 BHE sections and geometry representation through CLN. Rectangles are groundwater cells, octagons are CLN Wells and the*
 192 *line connecting the bottom octagons is the CLN polyline.*

193 Additional enhancements have been applied to the BHE simulation process since the discussions in (Antelmi
 194 et al., 2021). Specifically, three characteristic parameters of the BHE are introduced in the numerical code:

- 195 - the U-pipe (i.e. high density polyethylene) thickness;
- 196 - the U-pipe thermal conductivity;
- 197 - the internal convective heat transfer coefficient.

198 When the aim of the numerical simulation is to describe what happens into the BHE and the cells strictly
199 surrounding it, these parameters need to be considered. The enhancement improves the accuracy of the
200 numerical representation of the BHE and the heat transport between groundwater and BHE. The net thermal
201 resistance between aquifer and BHE is a sum of 2 resistances: the conductive resistance offered by the BHE
202 pipe wall and the convective one, related to the BHE circulating fluid. The latter is depending on the
203 convective heat transfer coefficient, that is linked to the inner diameter of the BHE tube, to the fluid flow
204 rate and regime (laminar or turbulent).

205 Another enhancement to the MODFLOW-USG software specific for the implementation of BHEs and the
206 simulation of a TRT was to provide appropriate boundary conditions to the inlet and outlet of the BHE tube
207 as discussed below.

208 2.2 Boundary conditions for the BHE

209 MODFLOW-USG includes several packages to provide boundary conditions to a simulation. These boundary
210 conditions can be applied to the GWF and/or the CLN domains. For instance, a flow rate and a temperature
211 may be provided at the inlet of the BHE tube and the code will compute the flow rate and temperature at
212 the outlet.

213 For a BHE, the outflow rate will be equal to the inflow rate, which may be applied as an outflow boundary
214 condition. If the flow in the BHE tube is at steady-state conditions, a reference head is required for a unique
215 solution to the flow in the BHE tube. Thus, a prescribed source flux may be provided at the inflow end. At
216 the outflow end, a reference head may be provided to allow the BHE fluid to exit (it can be any value above
217 the top of the model domain such that the tube remains fully saturated at the outlet point).

218 Typical operation of a TRT requires a constant heat rate injection. Thus, the temperature at the outlet of the
219 BHE is at a constant differential from the temperature at the inlet. The DRT package available in MODFLOW-
220 USG-Transport was modified to accommodate this condition. This package was developed to extract water
221 from cells characterized as a drain and re-inject all or part of it into another cell. This feature was expanded
222 for use with solute and heat transport problems: it allows to link the solute concentration, or temperature,

223 extracted from the drain cell (which can be the CLN cell representing the borehole outlet), with that of re-
224 injected water (into the CLN cell representing the borehole inlet).

225 By using the BHE outlet as a drain cell and the BHE inlet as a re-injection cell, it is possible to create a closed
226 loop circuit as in a TRT or in the common operation of a BHE. Since a reference head is required in the BHE
227 for a steady-state solution, an option is provided which allows for extraction of water under a Cauchy
228 boundary condition, which provides the reference head. In the DRT package file, the reference head and the
229 return flow rate are then set by the user and supplied to the BHE outlet and inlet CLN nodes, respectively, to
230 provide the appropriate flow within the BHE tube. This case is called the GHB-Q condition and is identified
231 by providing a negative conductance factor in the DRT package input file (Panday et al., 2013). The value is
232 converted to positive internally in the code.

233 A temperature difference (ΔT) can then be forced between the outflow and inflow such that the system
234 operates under a constant heat rate. The heating power actually depends on the mass flow rate of the heat
235 transfer fluid, on its heat capacity per unit mass and on the temperature difference ΔT . Since the mass flow
236 rate and the heat capacity are constant over time, ΔT is the only quantity that must be forced to remain
237 constant during the simulation. This requirement can be satisfied within the DRT input file, where a fixed
238 temperature increase can be added to the drained temperature before reapplying the water flow rate at the
239 return-flow location. This procedure allows an automatic implementation of the ΔT , thus overcoming the
240 method adopted so far with MODFLOW/MT3DMS, which required the simulation to be interrupted many
241 times to manually adjust this parameter.

242 Therefore, to properly use the DRT package, the following information must be introduced into the input
243 data file: the node number of the inlet and outlet cell of the BHE, the elevation of the water level for the
244 GHB-Q condition, the flux rate applied to the return flow node and the fixed temperature increase at the BHE
245 inlet node.

246 2.3 Numerical model implementation

247 Three main features are essential to numerically reproduce a conventional TRT:

- 248 1. the real pipe circular section of the BHE;

249 2. the circulation of the fluid inside the BHE;

250 3. a constant heat rate injection into the ground during the test.

251 When the numerical code involves only rectangular or square cells, such as MODFLOW and MT3DMS, the
252 circular geometry of the BHE must be approximated through an equivalence with a square or rectangular
253 one. Angelotti et al. used this approach with good results (Angelotti et al., 2014a), although with a big effort
254 in terms of computational load and implementation times: running the numerical model for one specific
255 groundwater flow velocity required more than 1 day for an expert user and a significant effort to find the
256 right combination of numerical solver parameters to achieve convergence. In specific, each square section of
257 the BHE pipe consisted of 36 cells, reproducing the heat carrier fluid, surrounded by 0.37 cm cells
258 representing the HDPE; the U-shaped elbow was implemented through two outer horizontal layers with a
259 thickness of 0.37 cm and one in the center of 3.36 cm.

260 Differently, in the present study the BHE is implemented in accordance with the approach proposed and
261 validated by (Antelmi et al., 2021) by means of three analytical elements: two CLN Wells representing the
262 inlet and outlet pipes and one horizontal CLN Polyline implementing the elbow of the U-tube. Since all these
263 elements are circular, this approach better reproduces the real geometry of the system, while the
264 unstructured grid approach allows to use a coarse grid (more details in subsection 2.4). Furthermore, as
265 already mentioned in subsection 2.1, the new version of CLN package, specifically updated for this study,
266 allows the user to include the HDPE thickness, although CLN elements are 1D, together with the HDPE
267 thermal conductivity and the convective heat transfer coefficient. The solver used for the numerical
268 simulations is the Sparse Matrix Solver (SMS), which includes a Total Variation Diminishing (TVD) scheme to
269 control numerical dispersion in the advection term. An adaptive time-stepping solution was selected,
270 automatically adapting the time step length to satisfy the Courant number constraints. The computational
271 time of each simulation is lower than 1 minute for any groundwater flow velocity (Intel(R) Core (TM) i9-9900K
272 CPU @ 3.60GHz).

273 In (Angelotti et al., 2014a), the authors simulated the constant heat rate operation of the BHE, maintaining
274 the heat carrier fluid circulation by means of Constant Head (CH) condition at the inlet and outlet of the U-

275 pipe and subdividing the total duration of the TRT into multiple simulations. During each simulation the inlet
 276 fluid temperature was defined as a function of the outlet fluid temperature at the last time step of the
 277 previous simulation using the equation:

$$T_{in_n} = T_{out_{n-1}} + \frac{Q}{mc_w} \quad (1)$$

278 where Q [W] is the constant heat rate injected into the ground, m [kg/s] is the mass flow rate into the BHE
 279 and c_w [J/ (kg K)] is the specific heat capacity of the heat carrier fluid.

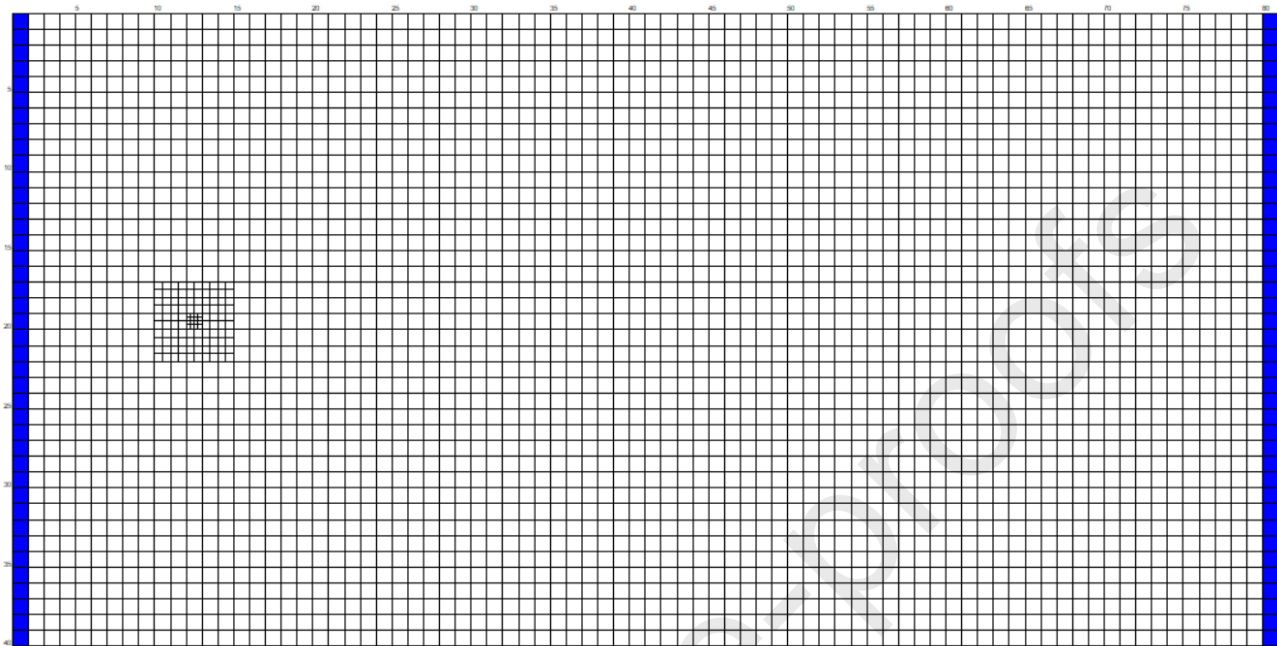
280 This manual methodology caused a high computational load and a significant loss of time to adapt each
 281 simulation. Differently, the new procedure here discussed leads to a rapid “automatic approach” using the
 282 DRT package for both circulating the heat carrier fluid and maintaining a constant heat rate injection during
 283 the test. The user needs to specify the flow rate circulating in the pipe (Table 1), the inlet and the outlet U-
 284 tube nodes where water is injected and extracted and the temperature difference to add to the fluid before
 285 its re-injection in order to maintain a constant heat rate of 40 W/m.

286 *Table 1 Geometric and operational properties of the BHE*

Property	Value	Measurement Unit
Flow rate	0.277	l/s
Depth	100	m
Inner radius	0.02	m
Pipe-to-pipe centers distance	0.06	m
HDPE thickness	0.0037	m

287 The case study implemented in MODFLOW-USG corresponds to the synthetic model discussed in (Angelotti
 288 et al., 2014a). It includes a BHE in a homogeneous saturated sandy and non-dispersive aquifer. The BHE
 289 features are provided in Table 1. The presence of the borehole filling material does not significantly influence
 290 neither the energy exchange nor the temperature profile into the aquifer (Alberti et al., 2017, 2016),
 291 therefore, the thermal properties of the grout material are assumed equal to the surrounding soil in both
 292 models. The dimensions of the modeling domain are equal to (Angelotti et al., 2014a), whereas the grid

293 discretization is different: the quadtree refinement is used (Figure 2) to refine the cells only in the proximity
 294 of the BHE as already applied in (Antelmi et al., 2021).



295

296 *Figure 2 Example of planar view of the numerical model domain; Constant Head condition is shown by blue cells.*

297 The groundwater flow direction is set through a Constant Head condition applied to the right and left
 298 boundaries cells and it results in West to East. The same boundary condition is assigned to set a constant
 299 unperturbed temperature equal to 11.8 °C, corresponding to the unperturbed temperature used in
 300 (Angelotti et al., 2014a). The thermal dispersion term is set equal to zero since dispersion is generally
 301 neglected for the heat transport in aquifer and is not even implemented into analytical solutions.
 302 Hydrological and thermal properties of the model, from (Angelotti et al., 2014a), are listed in Table 2.

303

Table 2 Hydrogeological and thermal properties implemented in the model in MODFLOW-USG

Parameter	Value	Measurement Unit
Hydraulic gradient, i	$4.97 \cdot 10^{-3}$	-
Aquifer horizontal hydraulic conductivity, K_x	$2 \cdot 10^{-5} - 2 \cdot 10^{-3}$	m/s
Aquifer vertical hydraulic conductivity, K_z	$2 \cdot 10^{-6} - 2 \cdot 10^{-4}$	m/s
Groundwater Darcy velocity, v	$0, 10^{-7}, 10^{-6}, 10^{-5}$	m/s
Aquifer porosity, Φ	0.35	-
Aquifer Specific Storage, S_s	0.01	m^{-1}

Bulk density, ρ_b	1700	kg/m ³
Solid specific heat capacity, c_s	747	J/(kg·K)
Water specific heat capacity, c_w	4154.2	J/(kg·K)
Solid heat conductivity, λ_s	3.18	W/(m·K)
Water heat conductivity, λ_w	0.59	W/(m·K)
HDPE heat conductivity, λ_{HDPE}	0.38	W/(m·K)
Convective heat coefficient, h	1137.39	W/(m ² K)
BHE mass flow rate, m	0.277	kg/s
Constant design heat rate	40	W/m
Longitudinal, Vertical, Transversal Dispersivity	0	m

304 2.4 Grid sensitivity analysis for different Darcy velocities

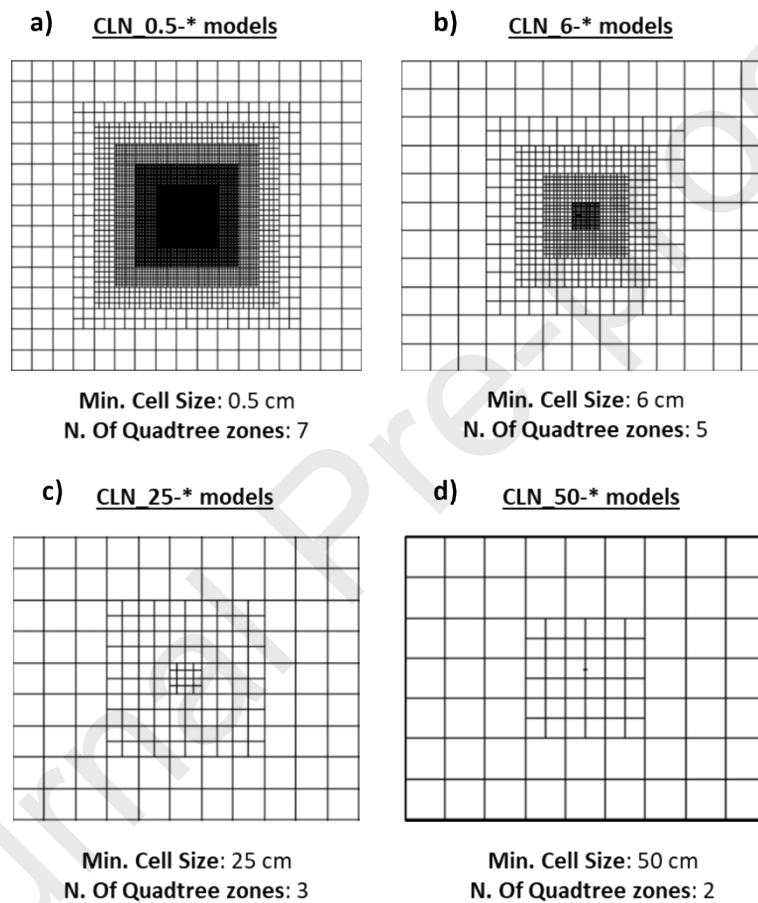
305 The added value of this research depends not only on the innovations to the DRT and CLN packages in
 306 MODFLOW-USG, but also crucially on the different grid refinements tested to achieve the best solution under
 307 different velocity regimes. A total of 16 different models are implemented combining 4 minimum cell size
 308 values and 4 Darcy velocities. Numerical model's nomenclature and characteristics are listed in Table 3.

309 *Table 3 Numerical models implemented*

V_{Darcy} [m/s]	V_{Darcy} [m/s]			
	0	10⁻⁷	10⁻⁶	10⁻⁵
Min cell size [cm]	Min cell size [cm]			
0.5	CLN_0.5-0	CLN_0.5-7	CLN_0.5-6	CLN_0.5-5
6	CLN_6-0	CLN_6-7	CLN_6-6	CLN_6-5
25	CLN_25-0	CLN_25-7	CLN_25-6	CLN_25-5
50	CLN_50-0	CLN_50-7	CLN_50-6	CLN_50-5
0.37	MA	MA	MA	MA

310
 311 The horizontal grid is characterized by a local refinement around the BHE implemented through a Quadtree
 312 approach, with a minimum cell size inside the refinement box ranging from 0.5 cm (Figure 3a) to 50 cm (Figure
 313 3d) and a maximum one outside the box ranging between 32 cm (Figure 3a) and 100 cm (Figure 3c, d).

314 Quadtree refinement is a straightforward way to focus resolution in areas of interest implementing a finer
 315 grid with different levels of detail (Panday et al., 2013). The user can specify a maximum number of seven
 316 concentric zones where the starting grid of the model is refined with a degree of detail increasing with the
 317 number of the zones (Antelmi et al., 2021). The two CLN Wells are implemented in two different adjacent
 318 cells to avoid numerical issues and as they do not need to be placed at the grid nodes but can be placed at
 319 any coordinate, it is possible to maintain a pipe-to-pipe centers distance of 6 cm for any grid geometry.



320
 321 *Figure 3 Detail of the plan view of the grid refinement implemented in the numerical models*

322 Each model consists of 20 layers with a thickness of 9 or 10 m for a total thickness of 200 m. Clearly, the
 323 model thickness was set greater than the BHE length (100 m) to avoid any influence of the bottom boundary
 324 condition which is a no flow and no energy exchange type. The first layer and the one containing the CLN
 325 Polyline (the tube elbow) thickness is about 1 m. The refinement in correspondence of these two layers
 326 proved to be fundamental to apply the 40 W/m required thermal power. The applied groundwater flow

327 velocities values vary from 0 to 10^{-5} m/s, to reproduce the typical range of velocities in hydrogeological
 328 natural systems.

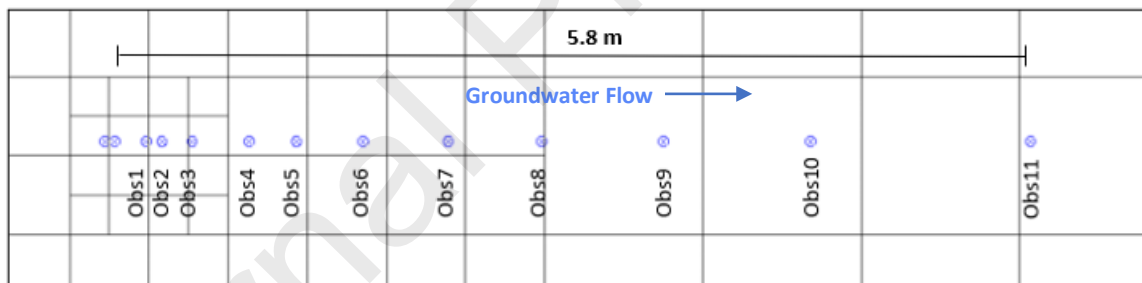
329 The TRT usually lasts no more than 72 hours, but here longer durations are simulated (up to 60 days). This is
 330 consistent with the study performed by (Angelotti et al., 2014a), where the duration was chosen to achieve
 331 steady state conditions in the aquifer temperature field.

332 2.5 Numerical model validation

333 (Brunetti et al., 2017)(Brunetti et al., 2017)The numerical model is validated by comparison with analytical
 334 results obtained from ILS and MLS approaches, as done in (Angelotti et al., 2014a).

335 To verify the accuracy and validate the 16 numerical TRT simulated in MODFLOW-USG, a comparison
 336 between the two approaches was conducted in terms of aquifer temperature values downstream of the BHE.

337 Temperature values are recorded at different time steps implementing 11 observation wells distributed at
 338 distances ranging from 0.2 m to 5.8 m from BHE-center (**Error! Reference source not found.**).



339
 340 *Figure 4 Detail of the modelling domain in one of the CLN_* models, containing the 11 monitoring wells*

341 Each monitoring well has a depth that reaches to the elbow of the heat exchanger; according to the choice
 342 of (Angelotti et al., 2014a) temperatures refer to a representative depth of 35 m.

343 The validation process aims to evaluate the divergence between numerical and analytical results in energy
 344 terms, through 4 steps:

- 345 1. evaluation through the numerical model of the aquifer temperature values in correspondence of 11
 346 monitoring wells (Figure 4) at different time steps: $T_{sub\ num}(x_i, y=0, t_k)$;
- 347 2. evaluation through the analytical models ILS/MLS of the aquifer temperature values downstream of
 348 the BHE: $T_{sub\ an}(x_i, y=0, t_k)$;

- 349 3. computation of the deviation between numerical and analytical solution in terms of Root Mean
 350 Squared Error (RMSE) at every time step;
- 351 4. minimization of the RMSE through the *fminsearch* Matlab function, using the specific heat rate in the
 352 ILS/MLS model as the minimization parameter. The achieved thermal power per unit length, named
 353 q_{fit} , along with the one simulated numerically q_{num} , allows to calculate an index of accuracy Δq of the
 354 numerical model, as in (Angelotti et al., 2014a). To evaluate the efficiency of the heat exchange of
 355 the new approach, thus further supporting the use of this tool for the typical operation of a BHE, the
 356 same index is here calculated as:

$$\Delta q = \frac{q_{fit} - q_{num}}{q_{num}} * 100 \quad (2)$$

357 For a complete view of the new suggested approach, the results are also discussed in terms of heat carrier
 358 fluid mean temperature and aquifer temperature, highlighting their dependence on the horizontal
 359 discretization and on the groundwater flow velocity implemented.

360 Extracting the temperature at the BHE inlet and outlet nodes and computing the arithmetic mean for each
 361 time step, the mean fluid temperature T_f is calculated as:

$$T_f(t_k) = \frac{T_{in}(t_k) + T_{out}(t_k)}{2} \quad (3)$$

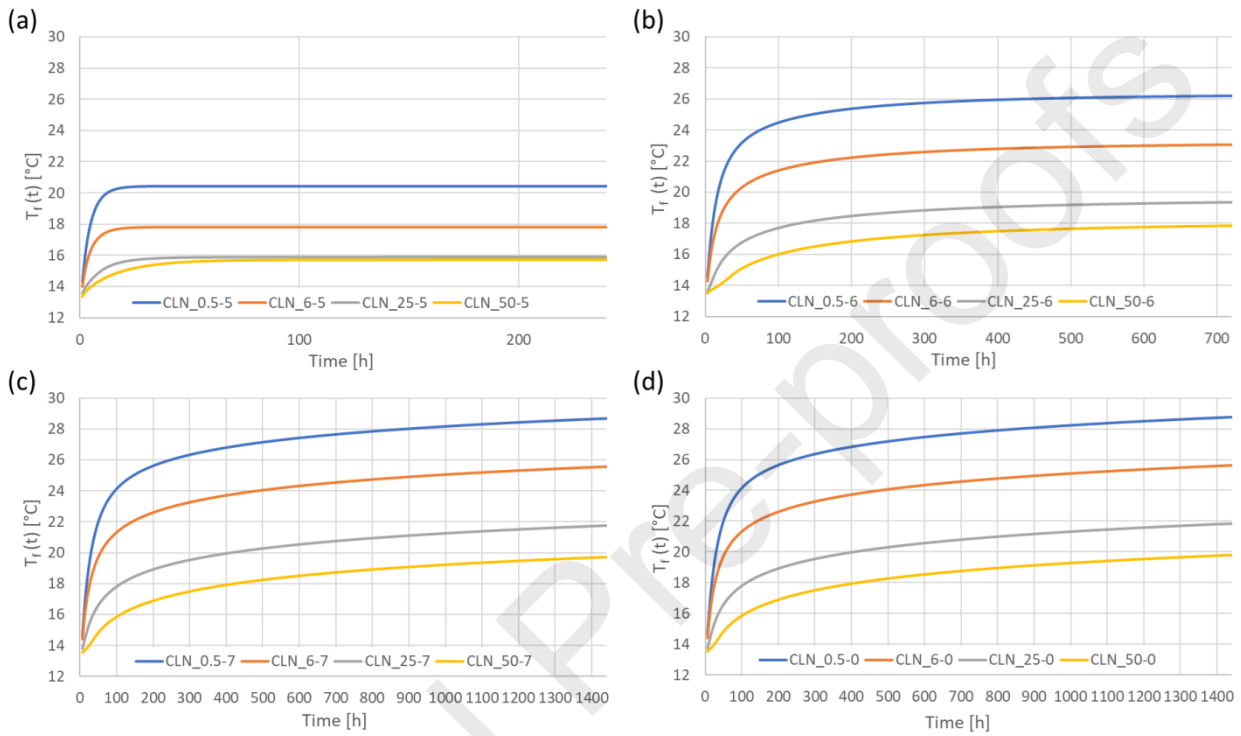
362 Finally, the results of the validation process are shown and compared with those achieved in (Angelotti et al.,
 363 2014a) through the “MA” models (Table 3).

364 3. Results and discussion

365 3.1 Heat carrier fluid mean temperature: grid sensitivity analysis for different Darcy velocities

366 The simulations were run under transient regime with different durations according to the different
 367 groundwater flow, as explained in subsection 2.4. From the results, an estimate of the heat carrier fluid
 368 temperature along the BHE depth, of the aquifer temperature downstream of the BHE and of the
 369 temperature variations during test time, were obtained.

370 The exchanged energy between BHE and aquifer was maintained constant and equal to 4000 W, by the
 371 regulation of inlet and outlet cells at the first layer of the U-shape pipe. The heat carrier fluid temperature
 372 analysis along the BHE depth is essential to understand how the energy exchange between BHE and ground
 373 layers varies along the vertical.



374

375 *Figure 5 Heat carrier fluid mean temperature over time simulated with “CLN_*-5” (a), “CLN_*-6” (b), “CLN_*-7” (c) and “CLN_*-0”*
 376 *(d) models. For each groundwater velocity the impact of the numerical grid is shown.*

377 In Figure 5, the trend of the heat carrier fluid temperature (T_f) as a function of time is shown for Darcy velocity
 378 equal to 10^{-5} m/s (a), 10^{-6} m/s (b), 10^{-7} m/s (c) and null (d). Due to the change in horizontal grid discretization
 379 around the BHE, for a given groundwater flow velocity (e.g. 10^{-7} m/s, Figure 5c), lower fluid temperatures are
 380 found as the minimum cell size increases. Considering the models “CLN_*-5” (Figure 5a), related to Darcy
 381 velocity equal to 10^{-5} m/s, at the end of the simulation, T_f assumes values equal to 20.4, 17.8, 15.9 and 15.7
 382 °C respectively for minimum cell size equal to 0.5, 6, 25 and 50 cm. On the other hand, as a result of the
 383 change in the plume shape around the BHE, for a given minimum cell size (e.g. 0.5 cm) fluid temperatures
 384 increase as the Darcy velocity decreases. Clearly, the dependence of the mean fluid temperature on the grid
 385 refinement is non-physical, while the dependence on the Darcy velocity is physically based.

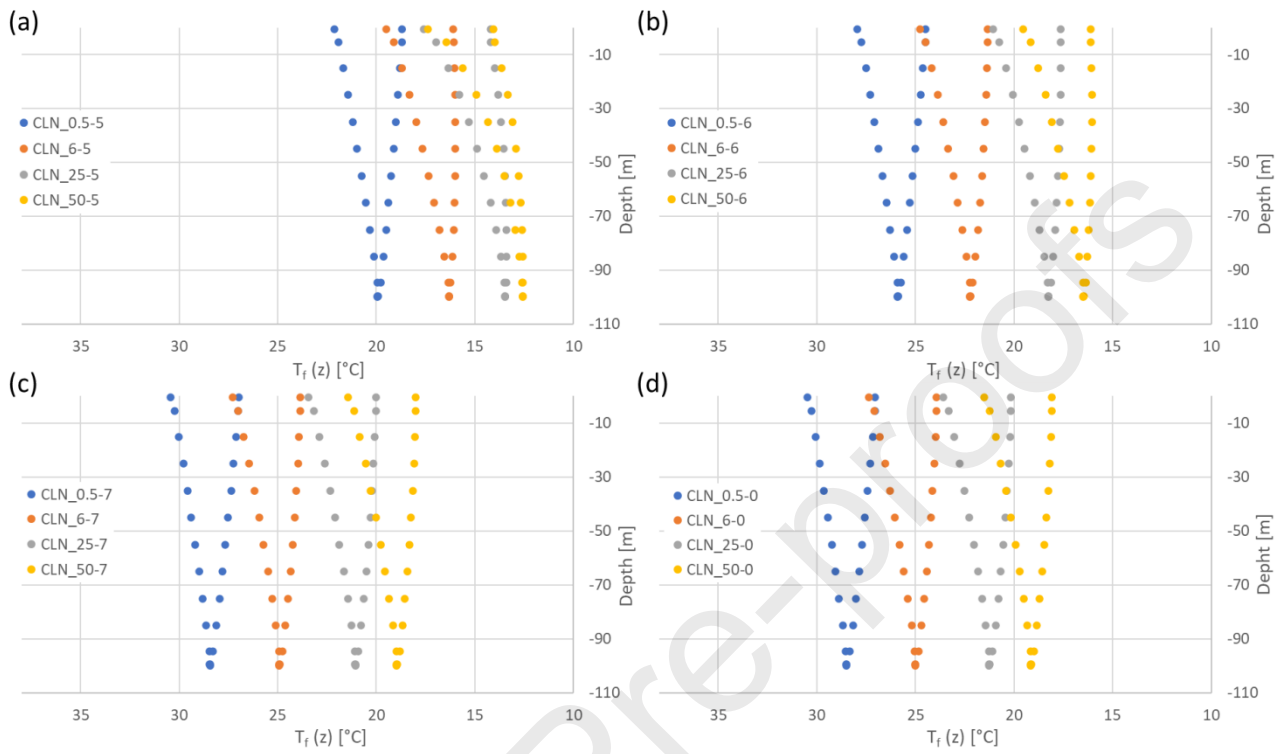
386 Table 4 shows the main results (heat carrier fluid mean temperature T_f , difference between inlet and outlet
 387 fluid temperature ΔT from BHE, specific heat rate q_{num} and variation from the design value of 40 W/m) at the
 388 last time step of each simulation.

389 *Table 4 Results obtained with the numerical simulations at the last time step in terms of heat carrier fluid mean temperature and*
 390 *simulated heat rate*

Groundwater velocity [m/s]	Min cell size [cm]	T_f at final time step [°C]	ΔT at final time step [°C]	q_{num} [W/m]	Variation from design q [%]
10^{-5}	0.5	20.42	3.44	39.41	-1.46
	6	17.79	3.42	39.30	-1.73
	25	15.91	3.39	38.99	-2.51
	50	15.72	3.34	38.47	-3.80
10^{-6}	0.5	26.22	3.45	39.16	-2.08
	6	23.06	3.43	39.19	-2.01
	25	19.35	3.43	39.32	-1.69
	50	17.82	3.42	39.33	-1.67
10^{-7}	0.5	28.71	3.44	39.05	-2.36
	6	25.58	3.43	39.09	-2.25
	25	21.74	3.43	39.27	-1.80
	50	19.71	3.43	39.35	-1.61
0	0.5	28.76	3.44	39.05	-2.37
	6	25.65	3.43	39.09	-2.25
	25	21.86	3.43	39.28	-1.79
	50	19.78	3.43	39.36	-1.58

391
 392 Despite the strong dependence of the heat carrier fluid temperatures on the horizontal discretization, the
 393 average heat rate per unit length q_{num} exchanged during the entire simulation differs by a few percentage
 394 points from the one imposed by the DRT package. A maximum deviation of -3.8% is obtained for the "CLN_50-
 395 5" model related to the greatest minimum cell size equal to 50 cm and to the maximum Darcy velocity.

396 The heat carrier fluid temperature distribution along the vertical, at the last time step for each numerical
 397 model (depending on flow velocity), is observed in Figure 6.

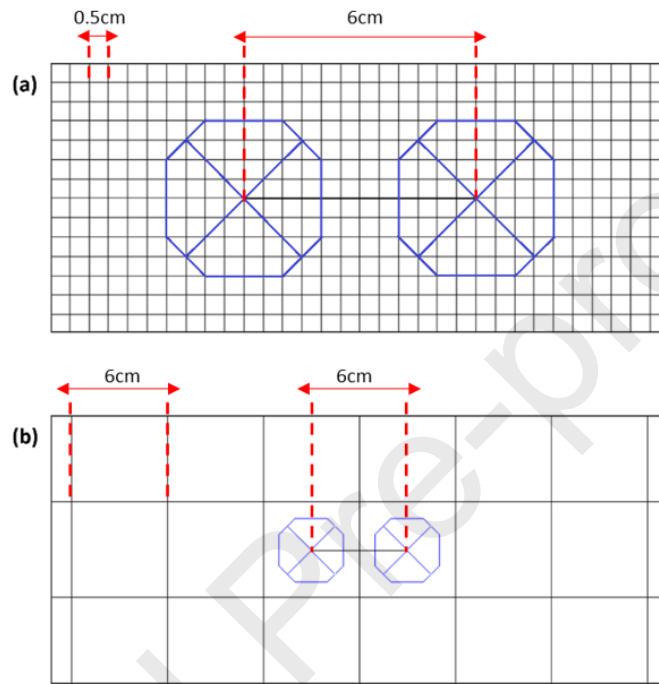


398

399 *Figure 6 Heat carrier fluid temperature as a function of depth after 10 days of constant heat rate injection for models “CLN_*-5” (a),*
 400 *30 days for models “CLN_*-6” (b), 60 days for models “CLN_*-7” (c) and “CLN_*-0” (d).*

401 The graphs display the temperatures of the delivery pipe on the decreasing branch of the curve (right side)
 402 and the ones of the return pipe on the increasing one (left side). As expected, the analysis confirms the
 403 behaviors described above: models with finer grids are characterized by higher temperatures (i.e. “CLN_0.5-
 404 *” and “CLN_6-*”); when a higher groundwater flow is implemented, at the same spatial discretization,
 405 temperatures are lower (i.e. “CLN_*-5” and “CLN_*-6”). The correct behavior of heat carrier fluid
 406 temperature as a function of depth should exhibit a decrease both during the descent and the ascent phases
 407 for any groundwater flow velocities. The Figure 6 shows that the models with groundwater flow velocity
 408 equal to 0 m/s and 10^{-7} m/s, for each grid discretization implemented, simulate the correct temperature
 409 distribution in the BHE. On the contrary, models with Darcy velocity equal to 10^{-5} and 10^{-6} m/s simulate heat
 410 transport less accurately for 25 and 50 cm size cases. In detail, temperature values along the return pipe stop
 411 decreasing as they proceed towards the ground level, assuming, in some cases, a constant temperature value

412 (“CLN_25-6” and “CLN_50-6”) or, in other cases, a progressively slightly increasing value (“CLN_25-5” and
 413 “CLN_50-5”). An explanation to this behavior can be achieved looking at the grid spacing. The heat exchange
 414 in the CLN domain is affected by temperatures calculated in GWF cells (outside the CLN cells area) located
 415 around the BHE; therefore, the implementation of different horizontal discretization leads to a different
 416 number of GWF cells between the delivery and return pipes of the U-shaped BHE (as shown in Figure 7).



417

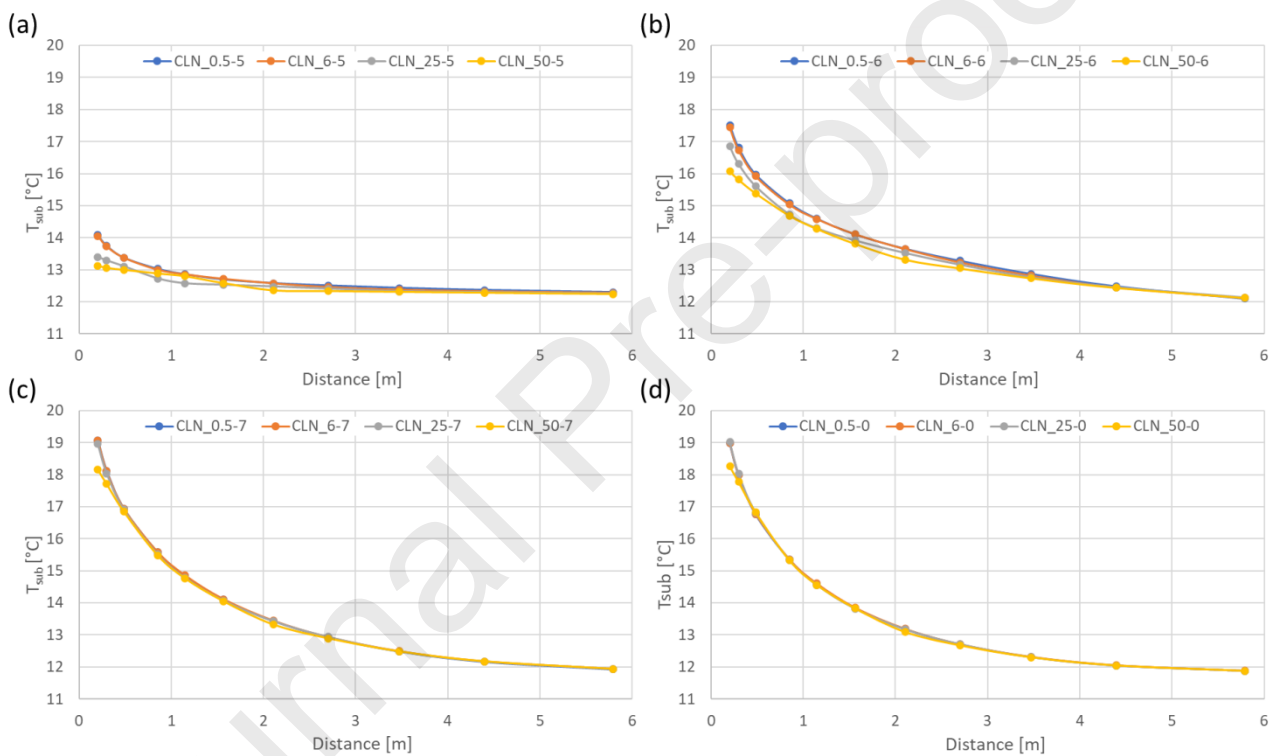
418 *Figure 7 Detail of the plan view of the modeling domain between the supply and return pipes into the “CLN_0.5-*” models (a) and*
 419 *into the “CLN_6-*” model (b)*

420 As shown in Figure 7, for models with a minimum cell size of 0.5 cm, 12 cells are present between the inlet
 421 and outlet pipes cells, whereas, for the remaining models, these CLN nodes are placed into two adjacent GWF
 422 cells. The presence of multiple cells between the two pipes provides an accurate interpolation between
 423 adjacent cells, able to detect the temperature increase occurring in that specific portion of the domain. Thus,
 424 the CLN nodes that identify the return pipe are in contact with colder cells than those around the delivery
 425 pipe, exchanging heat with the GWF domain nearby. This progressively decreases the heat carrier fluid
 426 temperature and provides a correct distribution of fluid temperature along the depth. On the other hand,
 427 when the U-pipe extreme cells are adjacent (Figure 7b) the heat exchange occurs between a very warm cell
 428 (inlet) and a very cold one (outlet) hindering an accurate simulation of the temperature distribution among

429 nodes inside the BHE. As expected, the behavior is more emphasized as the minimum cell size and the
 430 groundwater flow velocity increase.

431 3.2 Aquifer temperature: grid sensitivity analysis for different Darcy velocities

432 The horizontal thermal aquifer profile is reported in Figure 8, where temperature values are extracted at
 433 difference distances downgradient from the BHE in correspondence of 11 observation points, shown in Figure
 434 4, at the last time step of each simulation. This allows to analyze the groundwater thermal perturbation
 435 around the BHE. The constant heat rate injection for each simulation is defined in Table 4 (q_{num}).



436

437 *Figure 8 Aquifer temperature downstream of the BHE at 35 m depth, after 10 days of constant heat injection for model “CLN_*-5”*

438 *(a), 30 days for model “CLN_*-6” (b), 60 days for models “CLN_*-7” (c) and “CLN_*-0” (d), for each grid discretization.*

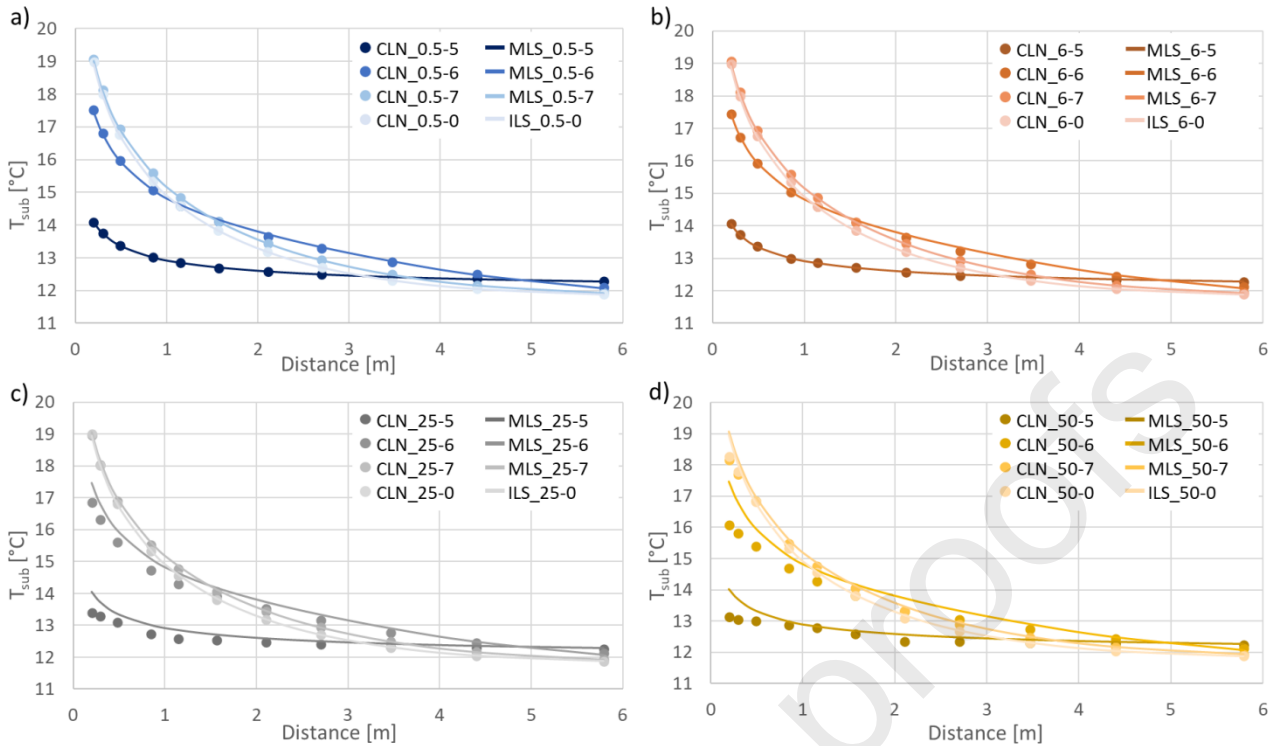
439 The graphs show that as groundwater flow increases (i.e. “CLN_*-5” and “CLN_*-6”), the thermal plume
 440 moves downstream more quickly, perturbing the aquifer even in the area farthest from the U-tube. Models
 441 with groundwater flow velocity equal to 10^{-7} and 0 m/s (i.e. “CLN_*-7” and “CLN_*-0”) show higher
 442 temperatures around the BHE and a less extended thermal plume, which leads to the natural groundwater
 443 temperature in the first meters downstream.

444 The horizontal grid discretization exerts an influence on aquifer temperatures, which is greater in the first 3
445 m downstream and in models characterized by a higher groundwater velocity. In detail, models more
446 affected by the spatial discretization are those with minimum cell size equal to 25 and 50 cm (“CLN_25-5”,
447 “CLN_25-6”, “CLN_50-5” and “CLN_50-6”). When groundwater flow velocity decreases, the influence of the
448 horizontal grid discretization is detectable only with models with a minimum cell size of 50 cm (“CLN_50-7”
449 and “CLN_50-0”).

450 Inside the GWF domain, the heat exchange computed between adjacent cells is strictly related to the
451 resolution of the model grid, as discussed for the heat carrier fluid temperature results. When the domain
452 grid is highly refined, the heat exchange between adjacent nodes is more precise, thus maintaining higher
453 temperatures around the BHE and simulating an accurate thermal plume regardless of the Darcy velocity
454 implemented in the model. In contrast, in wider grids, nodes are placed at greater distances, so temperature
455 values are averaged over larger cells. Therefore, these models are associated with globally lower aquifer
456 temperatures near the BHE, especially for advection-dominated models.

457 3.3 Validation against analytical solution

458 To assess the robustness of the new numerical modeling approach, a comparison with analytical solutions is
459 performed, such as discussed in literature. As already described in subsection 2.5, ILS and MLS analytical
460 solutions are implemented to perform a comparison both with the purely conductive and the advective case,
461 in terms of aquifer temperatures (Figure 9) and equivalent exchanged heat rate (Table 5). The constant input
462 heat rate value set in each analytical solution is the exchanged amount by the corresponding numerical
463 model (shown in Table 4 as q_{num}). This choice allows to compare groundwater temperatures when numerical
464 model and analytical solution have the exact same value of input heat rate. In Figure 9 the aquifer
465 temperature values are considered at the same domain points between numerical and analytical solution
466 (from 20 cm to 6 m downgradient of the BHE), for different groundwater flows. The results are shown at the
467 last time step of each simulation based on different groundwater flow velocities.



468

469

Figure 9 Aquifer temperature downstream of the BHE according to the MLS and ILS models and to the MODFLOW-USG simulations running "CLN_0.5-*" (a), "CLN_6-*" (b), "CLN_25-*" (c) and "CLN_50-*" (d) models.

470

471

For models with a minimum cell size of 0.5 cm and 6 cm (Figure 9a, b) a good agreement is achieved between the analytical and numerical temperature profiles for each groundwater flow velocity, with deviations lower than 0.2°C in absolute value. In contrast, models with a minimum cell size of 25 cm and 50 cm (Figure 9c, d) are associated with greater deviations. In particular, in Figure 9c higher errors are achieved near the BHE for higher Darcy velocities ("CLN_25-5" and "CLN_25-6"); Figure 9d shows larger deviations for all groundwater velocities, with greater errors associated with velocity of 10^{-5} and 10^{-6} m/s. The maximum deviation, equal to 1.4°C, is registered for model "CLN_50-6". These results are in accordance with those discussed in subsection 3.2: the main deviations between analytical and numerical results were found in "CLN_25-5", "CLN_25-6" and "CLN_50-*" models, less accurate in the first 2 m downstream of the BHE because of the wider grid discretization. Table 5 shows the results of the validation process in terms of q_{fit} and index of accuracy Δq previously defined (eq. 2).

481

482 Table 5 Results of the validation process in terms of q_{fit} and Δq achieved for the models implemented in MODFLOW-USG and the
 483 "MA" model

	10^{-5} m/s		10^{-6} m/s		10^{-7} m/s		0	
	q_{fit} [W/m]	Δq [%]	q_{fit} [W/m]	Δq [%]	q_{fit} [W/m]	Δq [%]	q_{fit} [W/m]	Δq [%]
CLN_0.5	39.5	0.3	39.2	0.1	39.2	0.4	39.3	0.7
CLN_6	39.0	-0.7	38.7	-1.3	39.2	0.3	39.4	0.7
CLN_25	30.2	-22.6	35.2	-10.4	38.7	-1.5	39.4	0.4
CLN_50	27.9	-27.4	31.9	-18.8	36.4	-7.4	37.5	-4.7
MA	36.4	-9.0	36.8	-8.0	39.5	-1.2	40.7	1.7

484 As expected, "CLN_0.5-*" and "CLN_6-*" models accurately simulate the constant heat rate injection results,
 485 regardless of the groundwater flow value implemented, producing a maximum relative discrepancy between
 486 q_{num} and q_{fit} , in absolute terms, equal to 1.3%. In energy terms, models with a minimum cell size equal to 0.5
 487 cm and 6 cm show an excellent agreement with the analytical solution both in the purely conductive case
 488 and in the advective ones. On the other hand, "CLN_25-*" and "CLN_50-*" models show higher percentage
 489 errors for groundwater flow velocity equal to 10^{-5} and 10^{-6} m/s, with a maximum overestimation equal to
 490 27.4%. Therefore, for the same models, a better agreement with the analytical solution is highlighted when
 491 the transport is mainly conductive.

492 Furthermore, the results in Table 5 show that "CLN_0.5-*" and "CLN_6-*" models reach a better agreement
 493 with the analytical solution than "MA" model, for all the analyzed groundwater velocities. The improvement
 494 is more noteworthy for the high Darcy cases, namely 10^{-6} and 10^{-5} m/s. Therefore, the new approach confirms
 495 and improves the results shown in (Angelotti et al., 2014a), although the simulation runtimes with the new
 496 techniques are shorter.

497 Although the validation process has shown errors below 5% even for "CLN_25-7", "CLN_25-0" and "CLN_50-
 498 0" models, the most suitable models for the TRT numerical simulation regardless of Darcy velocity, are the
 499 ones with a minimum cell size equal to 0.5 and 6 cm. Indeed, the use of minimum cell sizes ensures both to
 500 keep the heat rate constant over the time and to accurately simulate the heat exchange inside the aquifer
 501 and the U-pipe.

502 4. Conclusions

503 Over the past decade, progress achieved in numerical codes for simulating groundwater flow in porous media
504 and related processes led to an increasing use of numerical models as alternative tools to analytical ones for
505 Thermal Response Tests interpretation and typical BHE simulation.

506 Starting from the results discussed in (Antelmi et al., 2021), this study upgrades the MODFLOW-USG CLN
507 package in order to improve its capability in simulating BHE, and mainly focusing on the possibility to
508 implement a numerical TRT into the Control Volume Finite Difference. This has been achieved using a new
509 approach based on CLN and DRT packages. To support the study, the proposed methodology is tested
510 considering the detailed numerical model described in (Angelotti et al., 2014a) and well-known analytical
511 models (ILS and MLS). In the present study 16 numerical models are implemented by combining four
512 different Darcy velocities ranging from 0 to 10^{-5} m/s (representing a broad range of groundwater velocities
513 in aquifers), and four minimum cell sizes in the horizontal grid discretization around the BHE, ranging from
514 0.5 to 50 cm. Quadtree refinement around the BHE, a special tool to refine grid available for MODFLOW-USG,
515 is implemented to lighten the computational load. Each model implements a uniform, non-dispersive
516 geologic medium with the same hydrogeologic and thermal properties defined in (Angelotti et al., 2014a),
517 where a vertical BHE consisting of a single HDPE U-tube is implemented.

518 The results show that the new approach correctly simulates a constant heat rate operation, typical of a TRT
519 procedure, maintaining constant the exchanged heat rate between the BHE and the surrounding aquifer over
520 the time. For the more refined grid models, the average heat rate corresponding to the entire simulation
521 deviates less than 2% from the design heat rate imposed by the DRT package. Nevertheless, the
522 implementation of coarse grids can lead to an underestimation of the heat carrier fluid mean temperature
523 and, in the case of higher Darcy velocities, to an approximate heat exchange between the BHE and the
524 aquifer. Moreover, coarser grids tend to distort the profile of the thermal plume that develops in the first 2-3
525 meters downstream of the U-pipe. These results suggest that, for Darcy velocities higher than 10^{-6} m/s, the
526 grid refinement around the borehole radius should be on the order of 6 cm to accurately investigate the
527 thermal behavior of the aquifer in the first 3 m surrounding the BHE when conducting a TRT simulation. In

528 case of lower velocities, a grid size of 25 cm can be adequate. In fact, the validation process proved that
529 models with minimum cell sizes of 0.5 and 6 cm accurately simulate constant heat rate operation both in the
530 purely conductive case and for groundwater velocities between 10^{-7} and 10^{-5} m/s, while less stringent
531 refinements do not work optimally when the advective component is prevalent.

532 By way of contrast, when the aim of the study is mostly to assess the thermal impact in the aquifer beyond
533 3 meters downstream of the BHE, a refinement in-between 25 and 50 cm is appropriate. Moreover, since the
534 comparison with the results discussed in (Angelotti et al., 2014a) showed, for fine grids, lower errors for all
535 the Darcy velocities analyzed, a TRT implementation or a BHE standard operation in MODFLOW-USG allows
536 quicker, more efficient and accurate simulations than those performed in previous studies with MODFLOW
537 and MT3DMS. Overall, the results achieved confirm the issues discussed in (Al-Khoury et al., 2005; Florides
538 et al., 2012; Lamarche et al., 2010; Raymond et al., 2011; Signorelli et al., 2007): the implementation of a
539 pseudo-3D model lightens considerably the computational load of numerical models representing GSHP
540 systems, while guaranteeing a good accuracy in the results and providing the further possibility to implement
541 the operation of many BHEs within the same modeling domain.

542 Future developments of this study will result in applying the proposed method to the simulation of real-world
543 tests, either conventional or innovative (Enhanced TRT), to demonstrate its potential as a reliable TRT
544 interpretation tool. As the installation of GSHP systems will become more frequent according to the
545 decarbonization processes progressing in Europe, the results of the modeling approach presented will
546 provide efficient and reliable support in optimizing the design of geothermal borefields.

547 Finally, having lightened the computational load and demonstrated the good accuracy of the results, from
548 now on it will be possible to apply MODFLOW-USG to forecast the thermal impact of multiple geothermal
549 plants at community/urban scale, where many BHEs are operating. As in the major European cities these
550 energy systems are continuously growing, this will represent an important tool to identify potential
551 overlapping of thermal plumes, allowing the regulatory authorities to manage this underground energy
552 resource in a sustainable way, avoiding its over-exploitation over the foreseeable future.

553

Journal Pre-proofs

555 Nomenclature

Symbol	Variable [unit]
α	Thermal diffusivity [m^2s^{-1}]
C_m	Volumetric heat capacity of the medium [$\text{Jm}^{-3}\text{K}^{-1}$]
c_s, c_w	Specific heat capacity of solid and water [$\text{J}/(\text{kg}\cdot\text{K})$]
Δq	Index of accuracy for the validation process [%]
ΔT	Temperature difference between inlet and outlet fluid of the BHE [K]
D_l, D_t	Longitudinal and transversal thermal dispersion coefficient [m^2s^{-1}]
h	Convective heat coefficient [$\text{W}/(\text{m}^2\text{K})$]
i	Hydraulic gradient [-]
K_x, k_z	Hydraulic conductivity [m/s]
$\lambda_{\text{eff}}, \lambda_{\text{HDPE}}, \lambda_s, \lambda_w$	Effective thermal conductivity of medium, HDPE, solid and water [$\text{W}/(\text{m}\cdot\text{K})$]
m	Mass flow rate [kg/s]
Q	Heat rate [W]
$q, q_{\text{fit}}, q_{\text{num}}$	Specific heat rate, specific heat rate obtained with the interpolation process and simulated numerically [W/m]
ρ_b	Bulk density [kg/m^3]
R_b	Borehole thermal resistance [$\text{K}\cdot\text{m}/\text{W}$]
r_b	Borehole inner radius [m]
S_y, S_s	Specific yield [-] and specific storage [m^{-1}]
$T_f, T_{\text{in}}, T_{\text{out}}, T_o, T_{\text{sub}}$	Circulating fluid mean temperature, Temperature of the inlet/ outlet fluid of the BHE, Temperature of the undisturbed ground and Temperature of the subsoil [$^{\circ}\text{C}$]
t	Time [s]
v	Darcy velocity [m/s]

v_{eff}	Effective heat transport velocity [m/s]
Φ	Aquifer porosity [-]
BHE	Borehole Heat Exchanger
CLN	Connected Linear Network
COP	Coefficient Of Performance
DRT	Drain with Return Flow
GLHE	Ground Loop Heat Exchanger
GSHP	Ground Source Heat Pump
HDPE	High-Density Polyethylene
ILS	Infinite Line Source
MLS	Moving Line Source
TRT	Thermal Response Test
TSPEP	Two-Step Parameter Estimation Procedure

556

557

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- 703
- 704 - Improvement of CLN and DRT packages of MODLOW-USG for BHE numerical simulation
 - 705 - Testing of new procedure against previous numerical model and analytical solution
 - 706 - Possibility to reproduce typical GSHP system and Thermal Response Test operation
 - 707 - Easy and expeditious implementation of large borefield in a numerical model

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