Low temperature geothermal energy: heat exchange simulation in aquifers through Modflow/MT3DMS codes

Luca Alberti, Adriana Angelotti, Matteo Antelmi, Ivana La Licata, Cesare Legrenzi

Abstract: Geothermal energy and in particular low temperature resources, have a rising worldwide importance. Ground-Source Heat Pumps (GSHP) have been used increasingly because they are among the cleanest and most energy efficient heating and cooling systems for buildings. Simulation models can be applied for a more effective use of the subsoil for geothermal purposes. In fact they are useful tools for the design of efficient systems considering also the need to avoid abnormal temperature distributions in soil and aquifers.

In the hydrogeology field MODFLOW/MT3DMS are the most widespread programs to face environmental problems and to forecast quantity and quality impacts on groundwater resources. Although MODFLOW/MT3DMS are used to represent open circuit heat pumps, they are hardly used to represent borehole heat exchangers (BHE). The aim of this study is to simulate BHEs through two computer codes. The first one is TRNVDSTP, coupled to TRNSYS, which is often used in GSHP design in pure conduction cases. A methodology to take groundwater flow into account was added to TRNVDSTP, but a validation is still missing. The second one is MODFLOW/MT3DMS, suitable for groundwater flow and transport models, but whose reliability in BHE simulation is today unknown. The two software have been compared in terms of predicted exchanged energy and temperature distribution in the aquifer.

Keywords: Geothermal energy, Borehole Heat Exchanger, MODFLOW, MT3DMS, TRNSYS

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The first runs have been performed without a groundwater flow and a good agreement has been observed between the results of the two software, both in relation to exchanged energies and temperature distribution into the model domain.

Thus some simulations considering the presence of the groundwater flow have been performed. In this latter case the results in terms of exchanged energy differ of about 150%.

The study demonstrates the suitability of MODFLOW/MT3DMS for BHEs design when groundwater flow is not accounted for. Further efforts are needed to understand the different results when groundwater flow cannot be neglected, exploring the role of the different heat transport phenomena.

Riassunto*La risorsa geotermica ed in particolare lo sfruttamento del terreno come sorgente/pozzo termico a bassa temperatura stanno assumendo crescente rilevanza. Gli impianti a pompa di calore geotermica (GSHP) sono in continuo aumento poiché trattasi di una metodologia tra le più pulite ed efficienti dal punto di vista energetico per il raffrescamento ed il riscaldamento di edifici. Vi è la possibilità di sviluppare modelli di simulazione al fine di uno sfruttamento più efficace del terreno per scopi geotermici. Infatti tali modelli sono strumenti utili per la progettazione di sistemi efficienti che considerino anche la necessità di impedire lo sviluppo di temperature anomale in terreni ed acquiferi. Nel campo dell'idrogeologia i codici Modflow/MT3DMS sono tra i programmi più diffusi per affrontare problemi ambientali e prevedere dal punto di vista quantitativo e qualitativo gli impatti sulle risorse idriche sotterranee. Sebbene Modflow/MT3DMS vengano utilizzati per rappresentare pompe di calore a circuito aperto, essi sono ancora poco utilizzati per riprodurre sonde geotermiche (BHE). La ragione probabilmente risiede nel fatto che la rappresentazione della sonda geotermica attraverso questi codici richiede una geometria estremamente complicata ed un pesante raffinamento della griglia del modello. Lo scopo di questo studio è simulare le sonde geotermiche attraverso due codici di calcolo. Il primo è TRNVDSTP, associato a TRNSYS, il quale è spesso utilizzato per la progettazione di pompe di calore geotermiche in casi di sola conduzione. E' stata da poco aggiunta al codice TRNVDSTP una metodologia che considera la presenza di un flusso di falda, ma ancora non è stata convalidata. Il secondo codice è Modflow/MT3DMS, adatto per modelli di trasporto e per il flusso di acque sotterranee, ma la cui affidabilità nella simulazione di sonde geotermiche è oggigiorno sconosciuta. I due software sono stati confrontati dal punto di vista dell'energia scambiata e della distribuzione di temperatura previste nell'acquifero. Si è così implementata nei due programmi una sonda geotermica, costituita da un tubo ad U di lunghezza pari a 100 m e posizionata all'interno di un acquifero sabbioso saturo con spessore pari a circa 200 m. Si sono quindi eseguite simulazioni per il periodo di un anno al fine di rappresentare il funzionamento invernale ed estivo di una GSHP. Le prime simulazioni sono state effettuate senza considerare la presenza del flusso di falda e si è osservata una buona corrispondenza tra i risultati dei due software, sia dal punto di vista delle energie scambiate sia da quello della distri-*

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buzione di temperatura all'interno del dominio del modello. Pertanto sono state eseguite alcune simulazioni considerando la presenza di un flusso di falda. In questo ultimo caso i risultati in termini di energia scambiata differiscono di circa 150 %. I due codici di calcolo sembrano quindi simulare differentemente lo scambio termico tra il tubo ad U e l'acquifero e di conseguenza anche l'impatto del sistema geotermico sulle acque sotterranee. Il seguente studio dimostra che Modflow/MT3DMS è adatto per essere utilizzato nella progettazione di sonde geotermiche quando non viene preso in considerazione un flusso di falda. Si rende necessario però un lavoro maggiormente approfondito al fine di comprendere meglio i risultati differenti ottenuti in Modflow/MT3DMS e TRNVDSTP/TRNSYS qualora il flusso di falda non possa essere considerato trascurabile, indagando nel dettaglio il ruolo dei diversi fenomeni di trasporto del calore (conduzione, advezione, dispersione) al variare delle velocità del flusso di falda.

Introduction

Geothermal energy and in particular the use of low temperature resources has a rising worldwide importance (Lund et al. 2011). Ground-Source Heat Pump (GSHP) systems have been used increasingly because they are among the cleanest and most energy efficient heating/cooling systems for buildings. A typical vertical Borehole Heat Exchanger (BHE) consists of a number of boreholes, each containing a U-tube pipe in which a water/antifreeze solution is circulated. The depth of the borehole ranges usually between 40-150 m, and the diameter between 0.075-0.15 m. As shown in Figure 1, the BHE is coupled to the evaporator of the heat pump, allowing heat to be extracted from the ground and provided to the building. During summer, the operation can be reversed, so that heat is extracted from the building and injected into the ground.

Clearly the energy performance of GSHPs depends strongly on the heat transfer between the soil and the BHE. On the other side, from the hydrogeological point of view, one of the most important aspect in the use of GSHP systems is the forecast and control of the temperature in aquifer and groundwater and the development of the heat perturbation. From here the need to simulate, through mathematical models, the GSHP systems arises in order to evaluate the impact of temperatures in the subsoil.

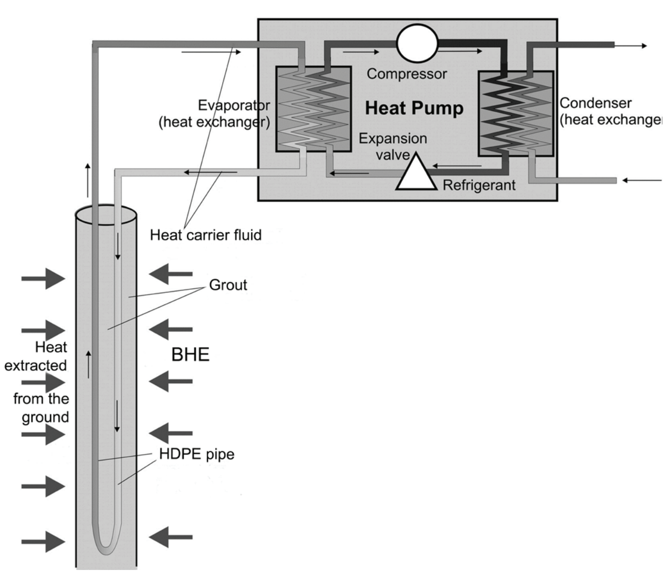

Fig. 1**:** *Operation of a GSHP in the heating mode*

A lot of efforts have been made to understand and to formulate the heat transfer process in the BHEs, resulting in several tools commercially available for design simulation of the BHEs. Among them TRNVDST (Hellstrom et al. 1995), coupled to the dynamic energy simulation software TRNSYS (Klein et al. 2004), is a widely used and reliable code, able to simulate the heat transfer process between the BHE and the ground as well as the thermal interaction among the different U-pipes. Most of the available tools, however, assumes pure heat conduction in the ground and doesn't consider the effects of a groundwater flow.

On the other side in the hydrogeology field there are lot of computer codes able to accurately simulate flow and mass transport in a variety of hydrogeological settings. The need to simulate the physical setting of a BHE is more and more increasing so some of the more used hydrogeological computer codes have been modified in order to be suitable to reproduce also heat transfer between BHE and aquifer. A new finite-element algorithm has been implemented in the commercial simulation code FEFLOW (Diersch, 2002) so that ground heat exchangers are modelled by a set of one-dimensional finite-element representations (Diersch et al. 2008). Among the finite differences computer codes MT3DMS (Zheng, 1999) is not explicitly designed to simulate heat transport, although temperature can be simulated as one of the species by entering appropriate transport coefficients. For SEAWAT (Langevin et al. 2003; Langevin and Guo 2006), a code designed to simulate coupled variable-density groundwater flow and solute transport, the ability to simultaneously model energy and solute transport is added representing temperature as one of the MT3DMS species (Thorne et al. 2006). Some of these codes and more in general numerical codes have been used in recent years to simulate BHEs operation in the presence of a groundwater flow (Chiasson et al. 2000, Fujii et al. 2005, Fan et al. 2007). The first two studies show that the groundwater effects on the BHE performance depend on the velocity and propose the use of the Peclet number to predict the relative importance of advection and thermal diffusion.

Fan (Fan et al. 2007) shows that groundwater flow increases the performance of the GSHP if the BHE is used only to absorb heat, while it leads to a worse performance if a daily charge/discharge operation strategy is adopted. In the above mentioned studies however the dispersion term seems to be disregarded in the heat transfer process. In a recent study by Hecht-Mendez et al. (2010) the suitability of MT3DMS to model GSHP systems is evaluated, by comparing the code results to analytical solutions and to other numerical codes. However in Hecht-Mendez et al. (2010) the BHE is simply modeled as a heat source with a given thermal power and therefore the U-pipe geometry and the heat carrier fluid are not described. Coherently the authors focus only on the temperature field generated by the BHE heat injection. A study on the suitability of MT3DMS to model a BHE, represented as a U-pipe with a given inlet fluid temperature, is still needed.

A few experimental studies on the impact of groundwater flow on the BHE operation can be found. Wang (Wang et al. 2009) measures the heat extraction rate of a BHE in the presence of a groundwater flow. However, the groundwater velocity is not directly measured but inferred from the measured vertical temperature profile in the ground. Moreover, in order to understand the role of the groundwater flow, the heat extraction rate of the BHE in the absence of flow

Tab. 1: *List of symbols and parameters used in the paper*

Symbol	Variable	Unit
C	Thermal capacity per unit volume	$J/(m^3K)$
C^k	Dissolved mass concentration	kg/m^3
C_s	Concentration of the sources or sinks	kg/m^3
c_s , c_w	Specific heat capacity of the solid or water	J/kg/K
$D*$	Molecular diffusion coefficient/Thermal diffusion coefficient	m^2/s
D_{ij}	Diffusion-dispersion tensor	m^2/s
Δt_i	Time step	S
θ	Volumetric water content	-
h	Convective coefficient	$W/(m^2K)$
K_d	Distribution coefficient	m^3/kg
k_{T0}	Effective thermal conductivity of the porous medium	W/(m×K)
k_{Tp} ,k_{Ts} , k_{Tw}	Pipe or solid or water thermal conductivity	W/(m×K)
I	Identity tensor	-
L	Side of the pipe represented by square section	M
L_c	Characteristic length	M
m_i	Mass flow rate at time *i*	Kg/h
π	Energy source/sink rate per unit volume	W/m^3
Q_i	Thermal power at time *i*	W
q_s	Volumetric flow rate per unit volume of aquifer representing sources and sinks	$m^3/s/m^3$
R	Thermal resistance per unit length	m×K/W
R_n	Retardation factor	-
r	Radius	M
r_b	Porous medium bulk density	kg/m^3
r_s , r_w	Density of the solid material or water	kg/m^3
s	Thickness	M
T, T_s	Temperature, temperature of the source	K
$T_{fin,i}$, $T_{fout,i}$	Heat carrier fluid inlet and outlet temperatures at time *i*	K
t	Time	S
v_i	Seepage velocity	m/s

has to be simulated through TRNSYS. A comprehensive hydrogeological characterization of the site where a real scale experiment is carried out in turn by Nam (Nam and Ooka, 2010). However the authors study the influence of the groundwater velocity on the energy performance of a Groundwater Heat Pump (GWHP) and not a GSHP. In general real scale experiments regarding real underground conditions would require a detailed survey of the hydrogeological conditions in order to be used either to validate simulation models or to assess the impact of a given groundwater flow. Clearly in real scale experiments parametric studies involving the groundwater flow conditions can hardly be performed.

The main aim of the present study is to assess the capacity of MODFLOW/MT3D to simulate a full BHE having a U-pipe geometry, in the absence of groundwater flow by comparing and discussing the results of two different codes, taken from the hydrogeology (MODFLOW/MT3D) and the energy fields (TRNSYS).

Different efforts are required by the two codes, both in the geometry description and in the calculation phase. On one side MODFLOW/MT3DMS is used. In order to reproduce the operation of a BHE coupled to a GSHP, an inlet fluid temperature is given as boundary condition to the U-pipe. The heat carrier fluid and the pipe geometry are described, and both the temperature field in the

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aquifer and the thermal power exchanged by the BHE are evaluated. On the other side TRNVDSTP (Pahud et al. 1996), a modified version of TRNSYS, is adopted. In TRNVDSTP a methodology to take groundwater flow into account has been introduced, although a validation is still missing. In turn its reliability in modelling the BHE operation, when only heat conduction in the ground is present, is well known. Therefore TRNVDSTP can serve as a reference to validate the MODFLOW/MT3DMS model in the absence of a groundwater flow.

Heat transport equation and implementation in MT3DMS

MT3DMS is a modular three-dimensional multispecies transport model for simulation of advection, dispersion, and chemical reactions of contaminants in groundwater systems (Zheng, C., Wang, P.P., 1999) and it represents the evolution of MT3DMS. MT3DMS can be used to simulate concentrations changes of miscible contaminants in groundwater considering advection, dispersion, diffusion and some basic chemical reactions, with various types of boundary conditions and external sources or sinks. MT3DMS can accommodate very general spatial discretization schemes and transport boundary conditions. MT3DMS is designed for use with any block-centered finite-difference flow model, such as the U.S. Geological Survey code named MODFLOW (McDonald MG, Harbaugh AW, 1996; Harbaugh et al, 2000).

The partial differential equation describing the fate and transport of contaminants of species k in three-dimensional, transient groundwater flow systems, disregarding chemical reactions, can be written as follows (Zheng and Wang, 1999):

$$\left(1+\frac{\rho_b K_d}{\theta}\right)\frac{\partial(\theta C^k)}{\partial t}=\frac{\partial}{\partial x_i}\left(\theta D_{ij}\frac{\partial C^k}{\partial x_j}\right)-\frac{\partial}{\partial x_i}\left(\theta v_i C^k\right)+q_s C_s^k \qquad [1]$$

where $\rho_b = (1-\theta)\rho_s$ is the bulk density and $K_d = \frac{c_s}{\rho_w c_w}$ is the distribution coefficient.

Even if MT3DMS was designed to simulate solutes transport, thanks to analogies between the heat transport and solute transport equation, the equation [1] can be rewritten considering temperature as one of the chemical species transported. Nevertheless in reason that the energy is transported and stored both by the fluid and the solid some adaptations are requested (D. Thorne et al., 2006), as explained below.

STORAGE: in equation [1] the left term accounts for changes in solute storage in aquifer matrix due to sorption processes. As heat is stored both in solid and liquid phase, both the specific heat capacity cs and cw have to be considered in the left side. Energy stored in the solid depends on temperature, solid volume, heat capacity and density: $(1-\theta)\rho_s c_s T$.

Similarly energy stored in the fluid phase is given by $\theta\rho_w c_w T$.

Thermal equilibrium has been assumed between the solid and the fluid phase. Then the storage term in the heat transport equation can be written as:

$$\left[\theta\rho_w c_w + (1-\theta)\rho_s c_s\right]\frac{\partial T}{\partial t} \qquad [2]$$

ADVECTION: considering the advection process for heat transport it is necessary to relate the temperature of the flowing water to the energy stored in the fluid. The energy can be calculated multiplying temperature by water density and specific heat capacity. As v_i is the volumetric flow rate per unit surface ((m^3/s)/m^2), multiplying it by ρ_w we obtain the mass flow rate per unit surface, that multiplied by water temperature and specific heat capacity gives us the advective heat flux in the flowing water: $\rho_w c_w v_i T$.

Therefore the advection term can be rewritten as:

$$\frac{\partial}{\partial x_i}\left(\rho_w c_w \theta v_i T\right) \qquad [3]$$

DIFFUSION-DISPERSION: in solute groundwater transport contaminants movement can be considered essentially limited to the liquid phase, whereas the energy is also transported through the solid by conduction process. This means that diffusion process can't be neglected for heat transport. As stated by the Fourier's law, assuming isotropic medium, the heat flux by conduction is given by

$$q_t = -k_{T_0}\frac{\partial T}{\partial x_j}.$$

For a saturated porous medium two different thermal conductivity values need to be used in the right term that accounts for diffusion-dispersion processes, namely k_{Ts} for solid phase and k_{Tw} for liquid phase, and an effective thermal conductivity is used:

$$k_{T_0} = \left[\theta k_{Tw} + (1-\theta)k_{Ts}\right].$$

Then a last adaptation is necessary for the dispersion transport because analogously to advective transport we need to relate the temperature of the "dispersed flowing" water to the energy stored in the fluid, which depends on density and specific heat capacity.

The term $\frac{\partial}{\partial x_i}\left(\theta D_{ij}\frac{\partial C^k}{\partial x_j}\right)$ in equation [1] is thus replaced by

$$\frac{\partial}{\partial x_i}\left(\left\{\left[\theta k_{Tw} + (1-\theta)k_{Ts}\right]I + \theta\rho_w c_w D_{ij}\right\}\frac{\partial T}{\partial x_j}\right) \qquad [4]$$

SOURCE/SINK: the last term in equation [1] represents the source or sink that adds or extracts solute mass from the system. Again for heat transport we need to take into account the energy stored in the fluid, so the new term is:

$$q_s \rho_w c_w T_S \qquad [5]$$

Consequently taking into account all the modifications above described, the heat transport equation can be written as (D. Thorne et al., 2006):

$$\frac{\partial}{\partial t}\left(\left[\theta\rho_w c_w+(1-\theta)\rho_s c_s\right]T\right)=\frac{\partial}{\partial x_i}\left(\left\{\left[\theta k_{Tw}+(1-\theta)k_{Ts}\right]I+\theta\rho_w c_w D_{ij}\right\}\frac{\partial T}{\partial x_j}\right)-\frac{\partial}{\partial x_i}\left(\theta\rho_w c_w v_i T\right)+q_s\rho_w c_w T_s \quad [6]$$

Notice that if there is no groundwater flow the pore velocity is null, so the advection and dispersion terms can be erased. Then equation [6] can be rewritten in the form of Fourier equation:

$$\left[\theta\rho_w c_w+(1-\theta)\rho_s c_s\right]\frac{\partial T}{\partial t}=\left[\theta k_{Tw}+(1-\theta)k_{Ts}\right]\frac{\partial^2 T}{\partial x_j^2}+\pi \quad [7]$$

where π is the energy source/sink term (W/m^3).Considering the equation [6], by dividing all the terms by $\rho_w c_w$ we obtain:

$$\left[1+\frac{(1-\theta)\rho_s c_s}{\theta\rho_w c_w}\right]\frac{\partial(\theta T)}{\partial t}=\frac{\partial}{\partial x}\left(\theta\left[\frac{k_{T_0}}{\theta\rho_w c_w}+D_{ij}\right]\frac{\partial T}{\partial x_j}\right)-\frac{\partial}{\partial x_i}\left(\theta v_i T\right)+q_s T_s \quad [8]$$

By introducing the bulk density ρ_b, the distribution coefficient K_d and the diffusion coefficient D^* as in the following equations:

$$\rho_b=\rho_s(1-\theta) \quad [9]$$

$$K_d=\frac{c_s}{\rho_w c_w} \quad [10]$$

$$D^*=\frac{k_{T_0}}{\theta\rho_w c_w} \quad [11]$$

the equation [8] may be rewritten in a form where the input parameters necessary for MT3DMS implementation are shown:

$$\left[1+\frac{\rho_b K_d}{\theta}\right]\frac{\partial(\theta T)}{\partial t}=\frac{\partial}{\partial x}\left(\theta\left[D^*+D_{ij}\right]\frac{\partial T}{\partial x_j}\right)-\frac{\partial}{\partial x_i}\left(\theta v_i T\right)+q_s T_s \quad [12]$$

TRNVDSTP/TRNSYS

The second simulation code adopted is TRNVDSTP coupled to TRNSYS 16. TRNSYS is a widely used dynamic simulation tool for thermal and electrical energy systems. It allows performing detailed analyses regarding energy performance and comfort conditions related to buildings and systems. A standard library provides a list of components ("types") representing common systems. User written or non-standard components may also be added, due to the modular structure of the code.

TRNVDSTP is a non-standard type that may be used to model BHEs. It is based on the Duct Storage Model (DST) developed at Lund Institute of Technology in Sweden (Hellstrom 1991). The DST combines numerical and analytical solutions to simulate the heat transfer process between the heat carrier fluid in the U pipe and the surrounding ground. Heat transfer in the ground is due only to thermal conduction and a cylindrical geometry is assumed. The model outputs regard the outlet fluid temperature, the thermal power exchanged by the fluid and the temperatures in the ground.

Due to its accuracy, the DST can be considered a reference for modelling BHEs.

In the TRNVDSTP version the effects on the BHE of a groundwater flow were included, by specifying a Darcy velocity for each ground vertical layer. The Darcy flow is used to calculate a convective loss from the so called "storage volume" to the surrounding ground, by means of forced convection correlations for a cylinder imbedded in a porous medium. However the method used to assess the influence of a regional groundwater flow has not been validated yet against accurate measurements or detailed simulations.

Case study

The case study refers to a typical BHE, consisting of a 100 m polyethylene U-pipe with an inner diameter of 2 cm and a pipe-to-pipe centers distance of 6 cm. The U-pipe is located into a 200 m saturated sandy aquifer, assumed homogeneous. For the sake of simplicity the borehole filling material is assumed to be equal to the surrounding soil. The BHE is simulated as if it was connected to a heat pump proving heating and cooling to a building in Milano. Therefore the aquifer has an initial uniform temperature of 11.8°C, that is representative of the annual average outdoor temperature for the chosen location. A water mass flow rate of 1000 kg/h is circulated into the U-pipe according to the annual time schedule reported in Table 2, where also the water inlet temperature is shown. Since the heat pump is not included in the simulation, a constant water inlet temperature is assumed, equal to 6°C in winter and to 30°C in summer. In the first simulation no groundwater flow was assumed and TRNSYS/TRNVDSTP was used as a reference for MODFLOW/MT3DMS. Then a set of simulations with a Darcy velocity equal to 10^{-6} m/s was carried out.

Tab. 2: *Operational parameters assigned to the BHE*

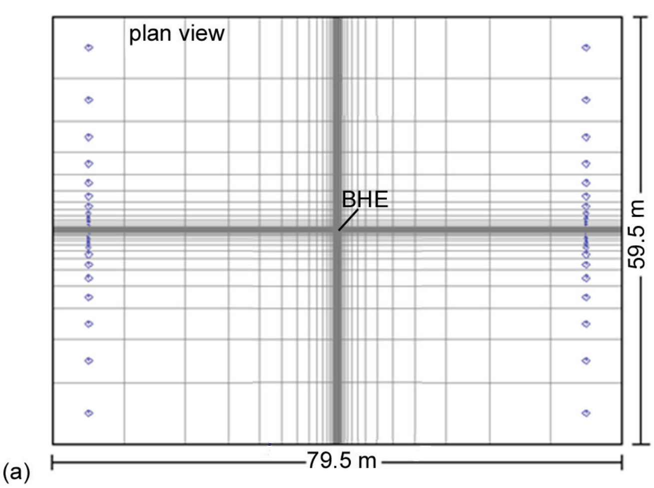
	First winter (1st Jan – 15th Apr)	First pause (16th Apr – 31st May)	Summer (1st Jun – 31st Aug)	Second pause (1st Sep – 15th Oct)	Second winter (16th Oct – 31st Dec)
Time [d]	105	46	92	45	77
T_{in} [°C]	6	-	30	-	6
Mass rate [kg/h]	1000	0	1000	0	1000

Model implementation in MODFLOW/MT3DMS

A simple three-dimensional model was implemented (Figure 2), in which active cells were assigned properties representing the aquifer and the inside of the pipe where the heat carrier fluid is assumed to circulate. Constant Head (CH = 100cm) and Constant Temperature (T = 11.8°C) were assigned to the left and right sides of the model domain (pointed cells in Figure 2a) and Initial T = 11.8°C was set to the entire domain.

The implementation of the real U-pipe geometry in MODFLOW/MT3DMS could require a significant computational effort. Therefore some simplifying assumptions were firstly adopted. The modelling then developed according to the following steps:

1. only the descending branch of the U pipe was represented and the thermal resistance of the plastic pipe was disregarded;
2. only the descending branch of the U pipe was represented but the pipe thermal resistance was taken into account;
3. the entire U pipe was described and the thermal resistance of the plastic pipe was considered



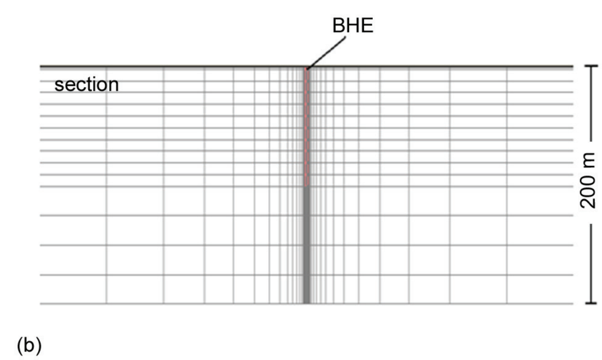


Fig. 2: *plan view (a) and section (b) of the model implemented in MODFLOW/MT3DMS.*

In all the steps, the problem of representing a pipe with circular section in MODFLOW/MT3DMS was faced. Actually in this code the grid consists of square or rectangular elements. Therefore the pipe was represented by a square section, whose size was derived on the assumption of keeping constant the total thermal resistance per unit length between the heat carrier fluid and the surrounding ground. This resistance is the sum of a convective resistance R_{cv} between the fluid and the inner surface of the pipe and a conductive resistance R_p given by the pipe, according to equation [13]:

$$R_{tot} = R_{cv} + R_p \quad [13]$$

In cylindrical geometry the convective and conductive resistances are expressed respectively by equations [14] and [15]:

$$R_{cv} = \frac{1}{2\pi r_{pi} h} \quad [14]$$

$$R_p = \frac{\ln(\frac{r_{pi}+s_p}{r_{pi}})}{2\pi k_{Tp}} \quad [15]$$

where the convective exchange coefficient between water and pipe h can be calculated by means of the Gnielinsky correlation for circular pipes (Incropera et al. 2007).

In plane geometry and discretizing the domain by a grid, the total thermal resistance from the fluid to the outside layer of the pipe R_{tot}', the convective resistance R_{cv}' and the conductive resistance R_p' are given by:

$$R_{tot}' = R_{cv}' + R_p' \quad [16]$$

$$R_{cv}' = \frac{1}{4Lh'} \quad [17]$$

$$R_p' = \frac{s_p'}{4L\lambda_p} \quad [18]$$

where the convective exchange coefficient h can be calculated again through Gnielinski correlation by adopting the hydraulic diameter $D_h = L$.

The aim is to hold the heat exchange coefficient constant, so it is necessary to impose:

$$R_{tot} = R'_{tot} \quad [19]$$

In step 1, where the pipe thermal resistance is disregarded, equation [19] means that the convective resistances should be the same. Following it was found that a circular pipe with an inner diameter of 4.00 cm is equivalent to a square pipe with a side of 4.09 cm. In steps 2 and 3, where the conductive resistance is included, by assuming also $s_p = s_p' = 3.7$ mm, equation [19] leaded to $L = 3.36$ cm for the equivalent square pipe side.

Once defined the correct dimension to represent the BHE size in MODFLOW/MT3DMS the horizontal grid across the borehole resulted as shown in Figure 3, Figure 4 and Figure 5c respectively for modelling steps 1, 2 and 3.

The parameters assigned to the aquifer and borehole cells in step 1 are listed in Table 3 with reference to Thorne et al. (2006). In order to hydraulically isolate the cells representing the pipe from the aquifer the Horizontal Flow Barrier (HFB) boundary condition was assigned to the polyethylene pipe walls (hydraulic conductivity: $1 \cdot 10^{-14}$ cm/d). A constant head boundary condition ($H = 100$ cm) was assigned to the pipe cell in the first layer while $H = 75.4$ m was set to the corresponding cell in layer 12 representing the bottom of the BHE at a depth of 100m, in order to correctly simulate the heat carrier fluid rate inside the pipe (1000 kg/h) that represents the usual operation rate.

One observation point (obs1) was located at 0.6 m from the pipes in order to monitor the simulated temperature. The distance of obs1 was set equal to the distance where TRNSYS gives its results.

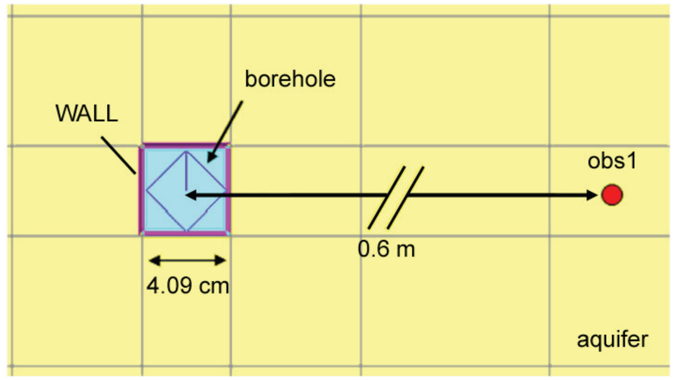


Fig. 3: *zoom on the center of the model domain in a Figure 2 to show the discretization across the cell representing the BHE in modelling step 1. Violet lines are WALL boundary conditions, the blue ones represents the CH assigned in layer1. Yellow color stands for aquifer while light blue is the inside of the pipes.*

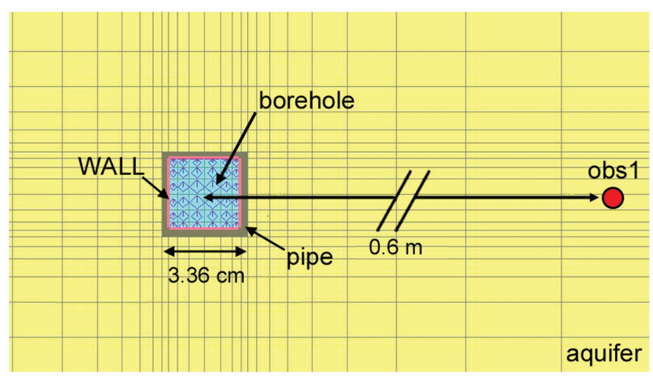


Fig. 4: *grid discretization across the BHE in modelling step 2. Violet lines are HFB boundary conditions, the blue ones represents the CH assigned in layer 1. Yellow color stands for aquifer while light blue is the internal part of the pipe*

In step 2 the pipe thermal resistance was taken into account and this required a model grid refinement to represent the correct polyethylene pipe thickness (0.37 cm). In order to respect the rule that the ratio between adjacent cells dimensions must be smaller than 1.5, the horizontal discretization appeared as indicated in Figure 4 and the number of cells representing the pipe became 36. The parameters assigned to the new zone representing the polyethylene pipe are listed in Table 4.

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Tab. 3: *Parameters assigned to the model in step 1; in Modflow/MT3DMS "Chemical Reaction" are used to define heat storage properties.*

Lenght [cm]	7950		
Width [cm]	5950		
Height [cm]	20000		
Number of rows	60		
Number of columns	77		
Column widths [cm]	3.36 – 1000		
Number of model layers	15		
Layer thickness [cm]	Layer 1: 100; layers 2-11: 1000; layer 12: 100; layers 13-16: 2500		
Hydraulic Conductivity	**Kx (cm/d)**	**Ky (cm/d)**	**Kz (cm/d)**
Aquifer	1.73E+03	1.73E+03	1.73E+02
Borehole	8.64E+08	8.64E+08	8.64E+08
Storage/Porosity	**Ss**	**Sy**	θ
Aquifer	0.01	0.20	0.22
Borehole	1	1	1
Dispersivity	**Longitudinal (cm)**	**Transverse (cm)**	**Vertical (cm)**
Aquifer	1000	100	10
Borehole	0	0	0
Chemical Reaction	**K_d (cm^3/g)**	**ρ_b (g/cm^3)**	
Aquifer	0.2	1.70	
Borehole	0.2	0.999	
Diffusion – Decay on soil	**D (cm^2/d)**		
Aquifer	1894.4		
Borehole	123		

Tab. 3: *Parameters assigned to the polyethylene pipe walls in modelling steps 2 and 3; in Modflow/MT3DMS "Chemical Reaction" are used to define heat storage properties*

Hydraulic Conductivity	**Kx (cm/d)**	**Ky (cm/d)**	**Kz (cm/d)**
Pipe walls	1.00E-14	1.00E-14	1.00E-14
Storage/Porosity	**Ss**	**Sy**	θ
Pipe walls	0.02	0.02	0.02
Dispersivity	**Longitudinal (cm)**	**Transverse (cm)**	**Vertical (cm)**
Pipe walls	0	0	0
Chemical Reaction	**K_d (cm^3/g)**	**ρ_b (g/cm^3)**	
Pipe walls	0.2	0.94	
Diffusion – Decay on soil	**D (cm^2/d)**		
Pipe walls	183		

Finally in step 3 the U-shape of the BHE was described (Tab.5) . A 3D representation of the BHE as implemented in MODFLOW/MT-3DMS is shown in Figure 5a and the new grid now appears as shown in Figure 5b and Figure 5c. The vertical discretization was modified to well represent the pipe "elbow": layer 13 (3.36 cm) represents the pipe, whereas layers 12 and 14 are 0.37 cm thick in order to assign the wall pipe properties described in Table 4. Constant head H = 100 cm is assigned in layer 1 to the left side cells representing the entrance of the U-pipe while H = 50.8 cm is set to the right side cells representing the exit of the U-pipe.

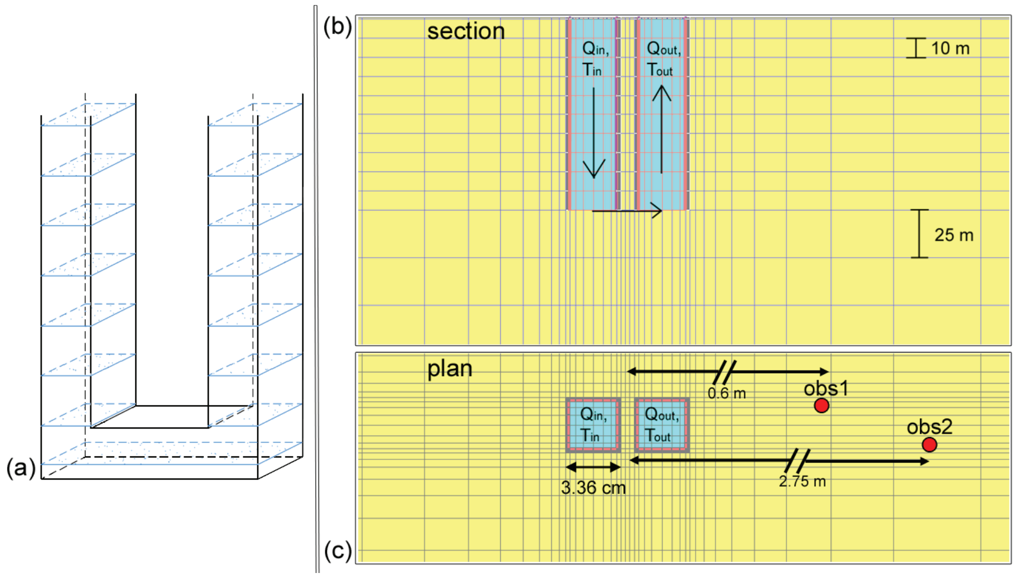

Fig. 5: *3D representation of the BHE in modelling step 3 (a); section (b) and plan view (c) of the new grid. In reason of their small thickness layers 12,13 and 14 are hardly visible. Yellow color stands for aquifer, light blue is the inside of the pipe and grey represents the BHE HDPE pipe. The distances of obs1 and obs2 are intended from the center of the U-shaped BHE.*

Tab. 5: *parameters assigned to the U-pipe model (modelling step 3).*

Lenght [cm]	7950
Width [cm]	5950
Height [cm]	20000
Number of rows	60
Number of columns	77
Column widths [cm]	3.36 – 1000
Number of model layers	18
Layer thickness [cm]	layer 1: 100; layers 2-11: 1000; layer 12: 0.37; layers 13: 3.36; layer 14: 0.37; layers 15-18: 2500

As an example, a plan and section view of the simulated temperature distribution obtained with modelling step 3 is shown in Figure 6.

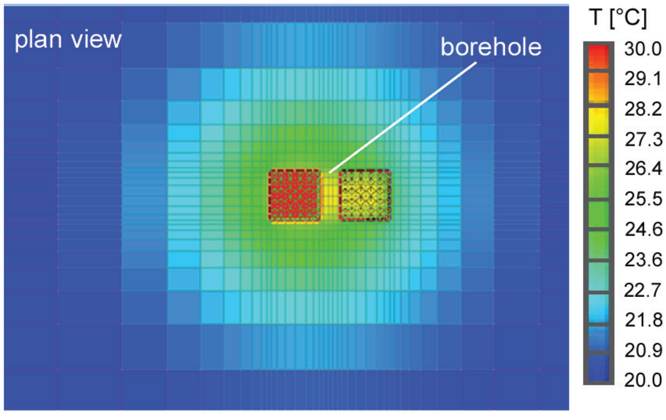

Fig. 6: *plan view of the simulated temperature distribution into the aquifer in modelling step 3 after 243 day.*

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Model implementation in TRNVDSTP/TRNSYS

The parameters required by TRNVDSTP are the U pipe geometry, the thermal properties of the saturated ground, of the heat carrier fluid and of the pipe material, the Darcy velocity and the initial ground temperature. Regarding the ground, an overall thermal conductivity k_{T0} = 2 W/(m×K) and an overall thermal capacity C_0 = 2.32 MJ/(m^3K) were assigned. These values are consistent with the bulk density, diffusion and distribution coefficient assigned to the aquifer in MODFLOW/MT3DMS and reported in Table 3. They represent weighted average values over the fluid and the solid portions in the saturated ground. The Darcy velocity was set equal to zero for the simulations without a groundwater flow and equal to 10^{-6} m/s for the case with groundwater flow. A uniform initial temperature equal to 11.8°C was assigned to the ground.

The time-depending inputs required by TRNVDSTP are the heat carrier fluid inlet temperature and flow rate and the ground surface temperature. The first two inputs were assigned according to the time schedule reported in Table 2. Contrary to MODFLOW/MT3DMS, an adiabatic condition at the ground surface cannot be specified in TRNVDSTP. Therefore, in order to minimize the heat exchange on the top and thus to reproduce as much as possible the MODFLOW/MT3DMS boundary condition, a constant temperature equal to the initial temperature 11.8 °C was assigned to the ground surface.

Simulations without a groundwater flow

As already mentioned, the two software were firstly compared in the purely conductive regime, where TRNVDSTP/TRNSYS provides reliable outputs. The comparison was carried out in terms of the predicted energy Q exchanged by the BHE during the heating/cooling season and of the calculated temperature distribution in the aquifer.

Q is given by equation [20]:

$$Q=\sum_i \dot{Q}_i\,\Delta t_i=\sum_i \dot{m}_i\,c_f\left(T_{fin,i}-T_{fout,i}\right)\Delta t_i \qquad [20]$$

The energy deviation σ_Q between the two software was then defined as in equation [21]:

$$\sigma_Q=\frac{Q_T-Q_M}{Q_T} \qquad [21]$$

where subscript T refers to TRNVDSTP/TRNSYS and subscript M refers to MODFLOW/MT3DMS.The mean square deviation in the temperature variation $\sigma_{\Delta T}$ was defined as in equation [22]:

$$\sigma_{\Delta T}=\sqrt{\frac{\sum_i\left(\Delta T_{T,i}-\Delta T_{M,i}\right)^2}{N}} \qquad [22]$$

where ΔT is the temperature variation in a given observation point in the aquifer compared to the undisturbed value and N is the total number of time steps for each period reported in Table 2.

A relative mean square deviation in the temperature variation $\sigma_{\Delta T}/\Delta T$ can also be usefully defined as in equation [23]:

$$\frac{\sigma_{\Delta T}}{\Delta T}=\frac{\sqrt{\dfrac{\sum_i\left(\Delta T_{T,i}-\Delta T_{M,i}\right)^2}{N}}}{\dfrac{\sum_i \Delta T_{T,i}}{N}} \qquad [23]$$

where the mean temperature variation calculated by TRNVDSTP/TRNSYS was chosen as a reference.

The results of the comparison are reported in Table 6. The energy deviation in the heating and cooling season are reported. The temperature variation deviations in each season refers to the two observation points shown in Figure 4c.

The results in Table 6 show the importance to consider the conductive thermal resistance of the pipe (look at the difference between step 1 and 2) and to model the whole U pipe rather than only the descending branch (see the difference between step 2 and 3). The comparison between steps 2 and 3 provides a sound indication of the energy exchanged by the ascending branch, which can account for up to 30% of the total energy exchanged by the U pipe. The difference between the two software tends to be larger for the temperature variation compared to the energy. The farther is from the U-pipe (observation point 2) the smaller is the temperature variation due to the BHE operation. Consequently in observation point 2 $\sigma_{\Delta T}/\Delta T$

Tab. 6: *Comparison between the two software without a groundwater flow*

	heating					cooling				
Modelling step	σ_Q	$\sigma_{\Delta T\ obs\ 1}$ (°C)	$\sigma_{\Delta T}/\Delta T$ obs 1	$\sigma_{\Delta T\ obs\ 2}$ (°C)	$\sigma_{\Delta T}/\Delta T$ obs 2	σ_Q	$\sigma_{T\ obs\ 1}$ (°C)	$\sigma_{\Delta T}/\Delta T$ obs 1	$\sigma_{T\ obs\ 2}$ (°C)	$\sigma_{\Delta T}/\Delta T$ obs 2
1	21 %	0.14	9%	0.22	63%	19%	0.18	4%	0.53	97%
2	-21%	0.39	33%	0.35	67%	-25%	1.60	31%	3.60	81%
3	6%	0.34	29%	0.14	24%	6%	0.92	20%	0.17	30%

tends to be larger than in observation point 1. However a good agreement between MODFLOW/MTD3DMS and TRNVDSTP/TRNSYS was found when modelling in MODFLOW the whole U pipe and the thermal resistance of the polyethylene pipe, as can also be seen in Figure 7 and Figure 8. Therefore, despite the strong mesh refinement resulted in lengthy run-times, the BHE representation adopted in modelling step 3 was chosen also for the next simulations, including a groundwater flow.

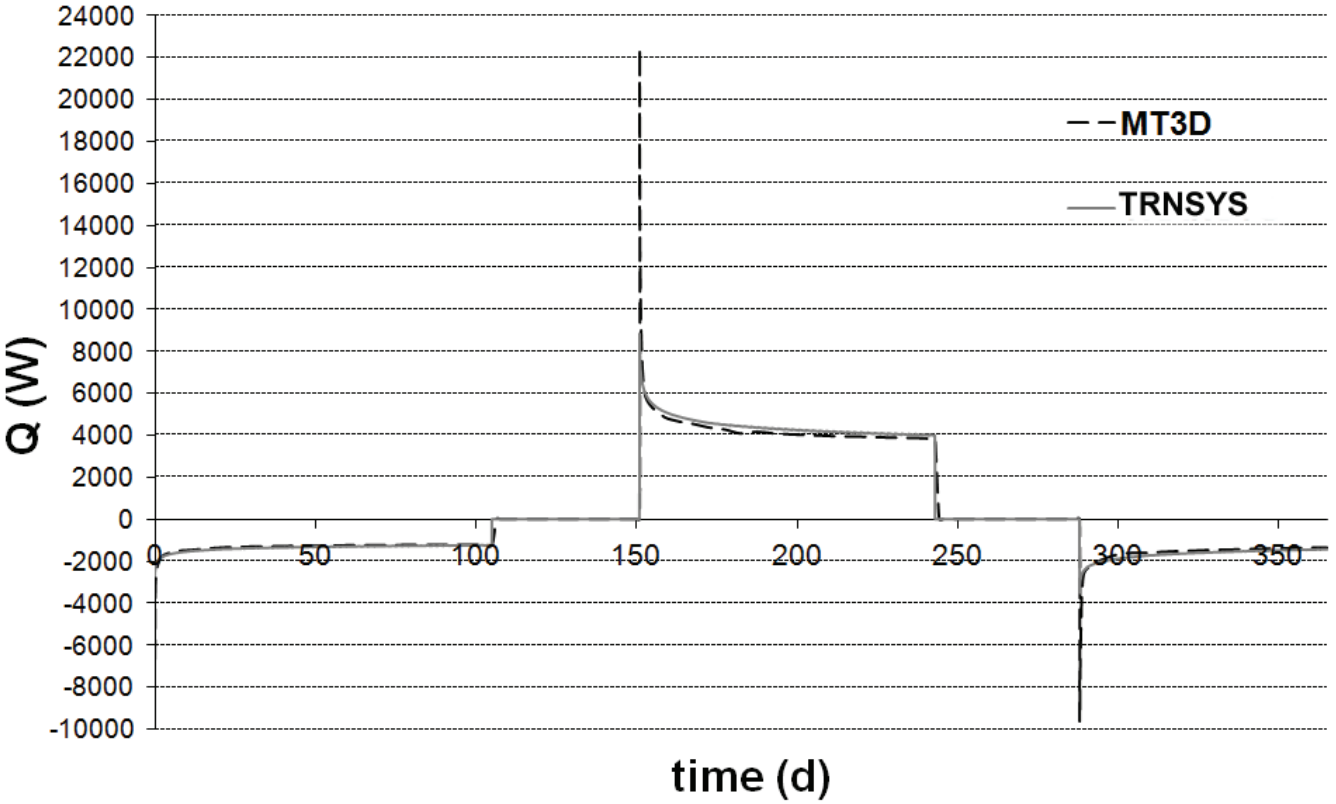

Fig. 7: *comparison of exchanged energy simulated by TRNSYS and MODFLOW/MT3DMS for one year (from Jan. to Dec.) in a saturated subsoil without groundwater flow.*

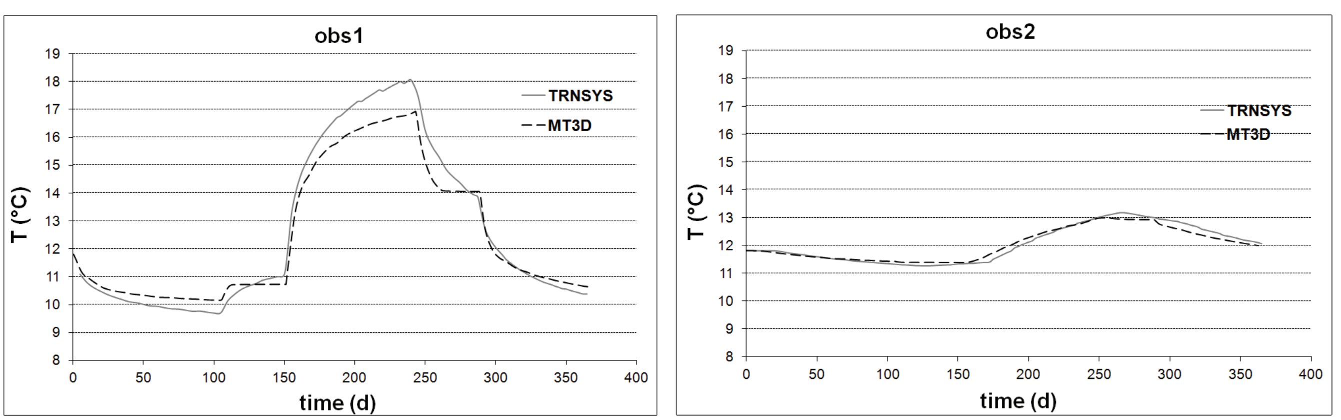

Fig. 8: *comparison of temperature simulated by TRNSYS and MODFLOW/MT3DMS in obs1 and obs2 for one year in a saturated subsoil without groundwater flow.*

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Simulations with groundwater flow

The simulated situation which does not account for a groundwater flow is representative of clay and silt hydrogeological units but can't be considered completely representative of the field conditions where BHEs are usually applied. Thus some simulations considering the presence of a groundwater flow, and maintaining the U-pipe geometry, were then performed. The groundwater Darcy velocity set for these simulations is 10^{-6} m/s corresponding to a gradient 0.5%.

In this case, the results in terms of exchanged energy for the two software differ of about 150% in both heating and cooling periods (Figure 8). In the two observation points (see Table 7) the mean square root deviation in the temperature variation increases also as a relative value, compared to the case without groundwater flow.

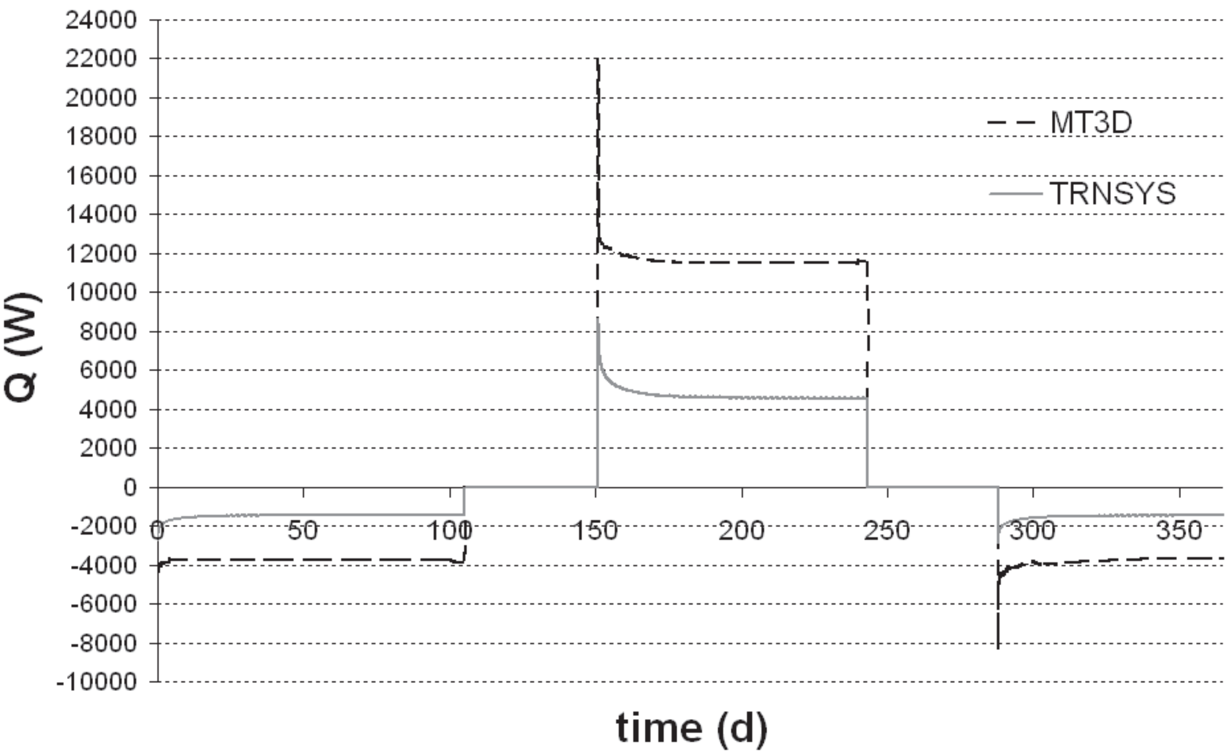

Fig. 9 : *comparison of exchanged energy simulated by TRNSYS and MODFLOW/MT3DMS for one year, considering a groundwater flow having a Darcy's velocity of $1 \cdot 10^{-6}$ m/s*

Tab. 7: *Comparison between the two software with a groundwater flow*

	σ_Q	$\sigma_{\Delta T\ obs\ 1}$	$\sigma_{\Delta T}/\Delta T_{obs\ 1}$	$\sigma_{\Delta T\ obs\ 2}$	$\sigma_{\Delta T}/\Delta T_{obs\ 2}$
heating	-149 %	0.70	51%	0.21	213%
cooling	-148 %	1.93	49%	0.78	174%

Moreover, a comparison in the exchanged energy between the case with a null groundwater flow and the case with groundwater flow can be carried out. According to TRNVDSTP/TRNSYS, the groundwater flow produces a modest increase in the exchanged energy, up to 14%. In turn in MODFLOW/MT3DMS a significant increase up to 162% was found.

Although a good agreement was found between the two codes with a null groundwater flow, they seem now to differently simulate the heat transfer between U-pipe and aquifer and then the impact of the geothermal system on groundwater.

Generally, neglecting groundwater flow, the heat transfer process is controlled by heat conduction. On the contrary, when the flow gradient is not null, the heat transfer process is also influenced by advection and dispersion. So the presence of groundwater makes the heat transfer process in the ground rather complex. Referring to the energy equation [12] it is possible to write it in a dimensionless form, allowing to highlight the physically homogenous quantities ruling the three heat transfer mechanisms present, namely D^* for conduction, D_{ij} for dispersion and $v_i L_c$ for advection, where L_c is a characteristic scale of the problem. In the present case study the ratio D_{xx}/D^* between the longitudinal dispersion and the diffusion coefficients is 2.1. By taking the BHE diameter as the characteristic length L_c, the ratio $v_i L_c / D^*$ between the advection term and the diffusion coefficient is 0.6. Consequently in this case the three heat transport mechanisms are all in the same order of magnitude and none of them can be considered dominant. Therefore in order to better understand the reasons of the observed discrepancy between the two codes, the authors will investigate further cases with a different relative importance of advection, dispersion and diffusion. Actually the two codes adopt different approaches in representing groundwater flow and heat transport. The MODFLOW/MT3DMS equation is more complete, in reason that the advection is fully calculated through the evaluation of the groundwater pore velocity and it consider both dispersive and diffusive transport mechanisms. Differently TRNSYS lacks in representing the dispersion term and the advection is represented in a less refined way.

Conclusions

Heat transport models are becoming more and more common to simulate borehole heat exchanger systems (BHE). This paper presents a comparison of numerical results between heat transport simulations of a BHE through two computer codes: the first one often used in GSHP design (TRNVDSTP, coupled to TRNSYS), the second one suitable for groundwater flow and transport models (MODFLOW/MT3DMS). Several simulations were performed to implement into the finite difference code the best configuration of the BHE that allows the best match of the results with TRNSYS ones. Initial attempts with simplified simulations have shown the need to fully implement in MODFLOW/MT3DMS the typical U-pipe geometry of a real borehole heat exchanger. In spite of the extensive computational resources and the complicated grid geometry necessary to represent the BHE, MODFLOW/MT3DMS shows to be able to well represent the fluid circulation into the pipe and the heat exchange with the aquifer for cases where groundwater flow is negligible. The comparison of simulations indicates a good agreement between the results of the two software, both in relation to exchanged energies, function of the fluid temperature inside the heat exchanger pipe, and temperature distribution into the model domain. In turn, when a groundwater gradient is applied, the two codes seem to differently simulate the heat transfer between U-pipe and aquifer and then the impact of the geothermal system on groundwater. At the moment on the basis of some consideration concerning the heat transport equation used by the two codes, MODFLOW /MT3DMS looks to be more suitable to represent cases where groundwater flow can't be neglected.

The authors are presently testing the results of some well-known analytical solutions in order to identify weakness and strength of the two codes when groundwater flow is important and fully understand the reasons of the pointed out differences. Further cases where the relative importance of diffusion, advection and dispersion is different from the case study presented here are being investigated.

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