PROCEEDINGS, 47th Workshop on Geothermal Reservoir Engineering
Stanford University, Stanford, California, February 7-9, 2022
SGP-TR-223

Coupling subsurface and above-surface models for optimizing the design of borefields and district heating and cooling systems in the presence of moving groundwater

Jianjun Hu, Christine Doughty, Patrick Dobson, Peter Nico, Michael Wetter

Lawrence Berkeley National Laboratory, Berkeley, CA, USA

{jianjunhu, cadoughty, pfdobson, psnico, mwetter}@lbl.gov

Keywords: Modelica Buildings Library, TOUGH, Borefields, District heating and cooling, Code coupling

ABSTRACT

Accurate dynamic energy simulation is important for the design and sizing of district heating and cooling systems with geothermal heat exchange for seasonal energy storage. Current modeling approaches in building and district energy simulation tools typically consider heat conduction through the ground between boreholes without flowing groundwater. While detailed simulation tools for subsurface heat and mass transfer exist, these fall short in simulating above-surface energy systems.

To support the design and operation of such systems, we have developed a coupled model including a software package for building and district energy simulation, and software for detailed heat and mass transfer in the subsurface. For the first, we use the open-source Modelica Buildings Library, which includes dynamic simulation models for building and district energy and control systems. For the heat and mass transfer in the soil, we use the TOUGH simulator. The TOUGH family of codes can model heat and multi-phase, multi-component mass transport for a variety of fluid systems, as well as chemical reactions, in fractured porous media.

In previous work, we described the coupling of these software packages, including how time-dependent boundary conditions for the borehole walls are synchronized for use in Modelica and TOUGH. We verified that the coupled Modelica/TOUGH code produced consistent results with the original Modelica code for an idealized problem in which heat transfer was purely by conduction in a uniform geologic medium. Here, we examine less idealized problems for which TOUGH's advanced capabilities for modeling fluid flow are required. The first example includes a thick vadose zone with a water-table depth that varies in time, which requires a fine vertical grid discretization for the 2D TOUGH model. The second example considers strong regional groundwater flow, which requires a 3D TOUGH model. Both examples require a new, more sophisticated coupling between the TOUGH and Modelica grids, which is described. Such models can be used to optimize borehole design and systems operations.

1. INTRODUCTION

Geothermal resources are considered a clean and sustainable form of renewable energy and have been utilized as the heating and cooling source and for thermal energy storage in district heating and cooling (DHC) systems. Simulation and optimization of DHC systems requires efficient and reliable models of the individual elements in order to correctly represent heat losses and gains, temperature propagation and pressure drops. When a geothermal borefield is present in the loop of the DHC system, the usual approach is to consider heat transfer in the subsurface to be purely by thermal conduction from the pipes to the surrounding soil and rock, with no consideration of fluid flow in the soil and rock. Coupling the DHC system to a subsurface model that can consider coupled fluid and heat flow loads in the soil and rock is still a challenge, which we address here through the coupling of the Modelica Buildings Library and the subsurface flow and transport simulator TOUGH.

The open-source Modelica Buildings Library (Wetter et al., 2014) developed by Lawrence Berkeley National Laboratory (LBNL), which includes dynamic simulation models for building and district energy and control systems, has models for closed-loop borefields (Picard and Helsen, 2014), based on so-called g-functions (Claesson and Javed, 2012). The models solve the transient heat flux in the ground by discretizing the ground surrounding the borehole in several cylindrical layers. The layer temperature at this outer radius is calculated using an approximation of the line-source theory together with superposition. However, this model assumes that heat transfer in the ground is purely by conduction, with no groundwater flow. TOUGH3 (Jung et al., 2018), the successor to TOUGH2 (Pruess et al., 2012), which was also developed by LBNL, simulates fluid flow and heat transport in heterogeneous geologic settings, including fractured rock, at scales ranging from core-scale to basin-scale. TOUGH considers multi-phase, multi-component fluid and heat flow in porous and fractured media. It employs the integral finite difference method for spatial discretization, enabling efficient, realistic representation of complex geologic and hydrologic features including grid layers that conform to tilted or warped beds, stochastic property assignments to represent highly heterogeneous formations, and local grid refinement. TOUGH incorporates accurate phase partitioning and thermophysical properties of all fluid phases and components. Various equation-of-state packages are available to represent different fluid combinations, such as the package EOS3, which considers components water and air, in liquid and gaseous phases, and is the relevant equation of state for aquifer or borehole thermal energy storage. The related code TOUGHREACT (Xu et al., 2014) adds the capability of including geochemical reactions, which may be added to the Modelica coupling in the future.

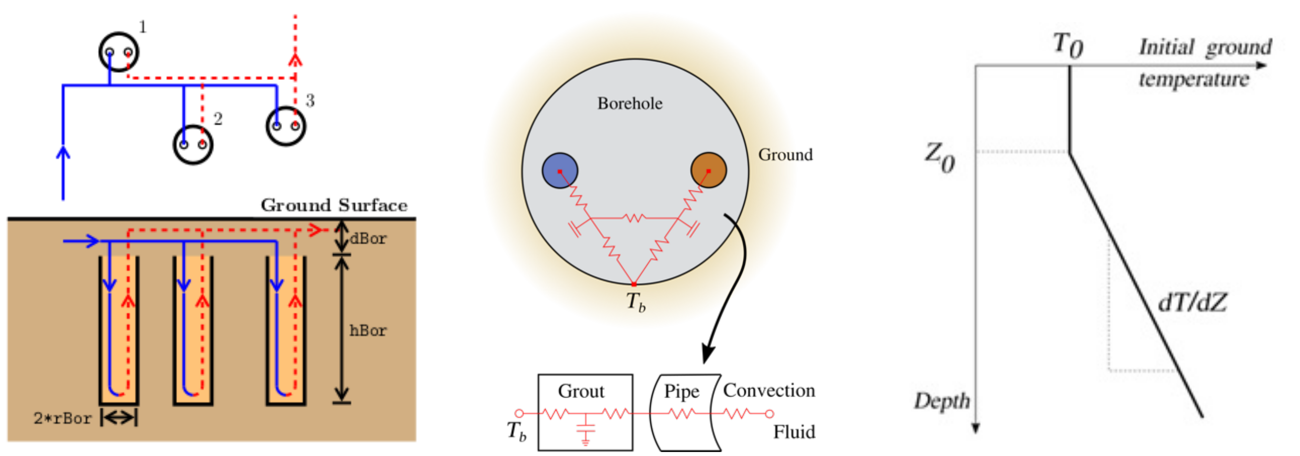
The key processes that TOUGH considers that are not included in the stand-alone Modelica treatment of the subsurface using g-functions may be divided into saturated-zone processes and vadose-zone processes. In the saturated zone beneath the water table, thermal conductivity and heat capacity may vary with local geology, and convective heat flow accompanies groundwater flow, which could be buoyancy flow arising from the injection of warm or cold water, or regional groundwater flow. In the vadose zone, thermal conductivity and heat capacity of rock with air-filled pore spaces are much smaller than those with water-filled pore spaces, and gas-phase flow involving water vapor and air may occur, greatly impacting surface heat transfer. Additionally, thermal properties would vary temporally with a changing water table, and latent heat effects accompanying evaporation or condensation could be significant for high-temperature systems.

In a previous paper (Hu et al., 2020), we presented a modeling approach to couple the above-surface DHC system modeling with Modelica and subsurface ground response modeling with TOUGH. We described the coupling approach and then validated it by applying the coupled model to the idealized case representing one borehole as a symmetry element within a large borefield, with uniform thermal conductivity and no fluid flow in the subsurface. We found that the coupled Modelica/TOUGH model produced results that agreed well with the original Modelica model incorporating g-functions. A subsequent paper (Doughty et al., 2021) presents a study considering a deep water table. The preliminary findings, which were based on TOUGH stand-alone simulations, show that even with a thicker vadose zone, and significant liquid- and gas-phase flow, but no regional groundwater flow, the borehole heat transfer problem remains insensitive to fluid flow. In the present paper, we revisit the deep water-table cases through Modelica/TOUGH coupled simulations. We then look into the effect of the regional groundwater flow on the borehole heat transfer and the performance of the district heating and cooling system. For both casas, we couple the TOUGH ground simulation with the district energy system that is modeled by Modelica (Hu et al., 2020). The simulated district energy system includes a sewage heat exchange station and the geothermal borefield in the loop as energy sources for three buildings: office, hospital and apartment. All Modelica models are available from https://github.com/lbl-srg/modelica-buildings, branch issue1495_tough_interface_moreIO_3D, commit c2a2d2a. The needed files for TOUGH simulation and the coupling interface are in the folder Buildings/Resources/Python-Sources.

2. BOREHOLE AND BOREFIELD GEOMETRY, AND BOREHOLE INLET BOUNDARY CONDITIONS

As in the previous study (Hu et al., 2020), we consider a DHC system with three building types (office, hospital, and apartment) and a sewage heat-exchange station, which includes a single-U-tube borefield as its cooling and heating source. We assumed that the borefield has following characteristics, illustrated in Figure 1 with parameters given in Table 1:

- Boreholes are connected in parallel.
- Boreholes are uniformly distributed and the distances *DBor* between them are the same.
- All boreholes have the same inlet water flow rate and temperature.
- All boreholes have the same length *hBor*, the same radius *rBor*, and are buried at the same depth *dBor* below the ground surface.
- The conductivity, capacitance and density of the grout and pipe material are constant, homogeneous and isotropic.
- Inside the borehole, the non-advective heat transfer is only in the radial direction.
- The borehole length is divided into multiple segments (*N*) and each segment has a uniform temperature.
- Horizontal heat transfer at the perimeter of the borefield with the undisturbed soil is negligible.
- Initial ground temperature has a profile as shown in Figure 1c.



a) b) c)

Figure 1: Assumptions used in this study: a) typical single-U-tube borefield, shown here with heat being extracted from the subsurface; b) thermal network of each borehole segment; c) initial ground temperature

Based on these assumptions, all boreholes within the borefield behave identically, so only one need be modeled. Within Modelica, the borehole is discretized along the depth z. Within each segment, the temperatures of the cool downward-flowing leg of the U-tube and the warm upward-flowing leg of the U-tube are modeled with circuit theory to produce a single temperature $T_b(z, t)$ representative of the borehole temperature for that segment (Figures 1a and 1b). It is $T_b(z, t)$ that is passed to and from TOUGH, along with the heat source/sink strength $Q(z, t)$, which is a function of time that depends on the energy supply and demand of the DHC system. The coupling is described in detail in Hu et al. (2020), but the basic idea is that Modelica calls TOUGH at time t_M for a fixed synchronization time step of duration dt_M, with $T_b(z, t_M)$ and $Q(z, t_M)$ specified. TOUGH then simulates the subsurface fluid and heat flow, using as many time steps dt_T as required to reach dt_M. Typically, $dt_T = dt_M$, but if complex flow processes are occurring, then $dt_T << dt_M$ is possible. TOUGH then returns $T_b(z, t_M+dt_M)$ to Modelica, which uses it until the next synchronization time step.

Table 1: Parameters and the values used for the borefield

Parameter	Value	Description
hBor	100 m	Height of the borehole
N	10	Number of borehole segments
rBor	0.075 m	Borehole radius
dBor	1.0 m	Depth of top of borehole
DBor	6.0 m	Distance between boreholes
dT/dZ	0.01 or 0.025 K/m	Vertical temperature gradient of undisturbed soil/rock
m_flow	0.02~0.24 kg/s	Water flow rate in the borehole
T_0	10 or 15°C	Surface temperature
Z_0	10 m	Depth below which temperature gradient starts

3. 2D DEEP WATER-TABLE CASES

The assumption of uniform thermal conductivity that was employed in previous studies (Hu et al., 2020) is not very good when a vadose zone exists, because thermal properties of dry or partially-saturated soil differ significantly from those of liquid-saturated soil. Our work (Doughty et al., 2021) looked into the effect of shallow and deep water tables. The TOUGH stand-alone simulations for a deep water-table did not show significant difference among studied cases. In this section, we further look into the deep water-table case (with depth around 50 meter) with a Modelica/TOUGH coupled simulation, in which Modelica simulates the above-ground district energy system (Hu et al., 2020). The grid used for the TOUGH simulation is the same as in Doughty et al. (2021), and has higher vertical resolution than does the Modelica representation of the borehole. Therefore, we average temperatures from the TOUGH model to assign to Modelica, and distribute temperatures from Modelica to assign to the TOUGH model (see Doughty et al. (2021) for more details).

Four cases are chosen to create a variety of fluid flow conditions. We consider both constant and time-variable water tables, and low (1E-13 m^2 = 100 mD) and high (1E-11 m^2 = 10 D) permeabilities (Table 2). We use van Genuchten (1980) relative permeability and capillary pressure curves, with Leverett scaling for capillary pressure, meaning the capillary fringe has different water content for low and high permeability cases. The two permeability values were chosen to provide saturated-zone Rayleigh numbers above and below the critical Rayleigh Number, so that natural convection is not expected for the low-permeability case, but is for the high permeability case. The sinusoidally varying pressure boundary at the bottom of the model as shown in Figure 2 creates a variable water table. For the constant water-table case, the pressure at the bottom model boundary is held fixed. The detailed case settings can be found in Doughty et al. (2021).

Table 2: Four simulation cases studying effects of deep water table

Cases	Permeability	Bottom pressure
1	low	Constant
2	low	Sinusoidal
3	high	Constant
4	high	Sinusoidal

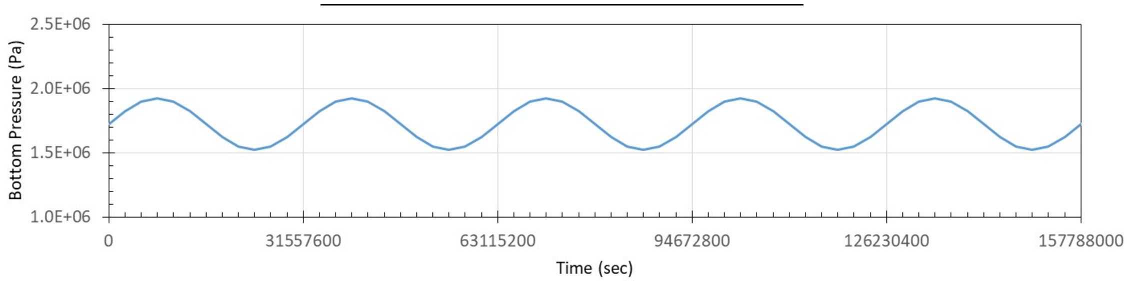


Figure 2: Pressure boundary condition assigned at the bottom boundary of the TOUGH model

3.1 Results

Figure 3 shows the temperature variation at various depths in the ground for a constant-depth water table, for cases with low and high permeability. With high permeability, the ground temperature at the borehole bottom and at the water-table depth becomes cooler at the year-end; the ground temperature at the capillary fringe shows larger fluctuations early in the year. This shows that higher permeability causes stronger heat transfer between the ground and the borehole, which is consistent with natural convection in the groundwater enhancing heat transfer to and from the borehole.

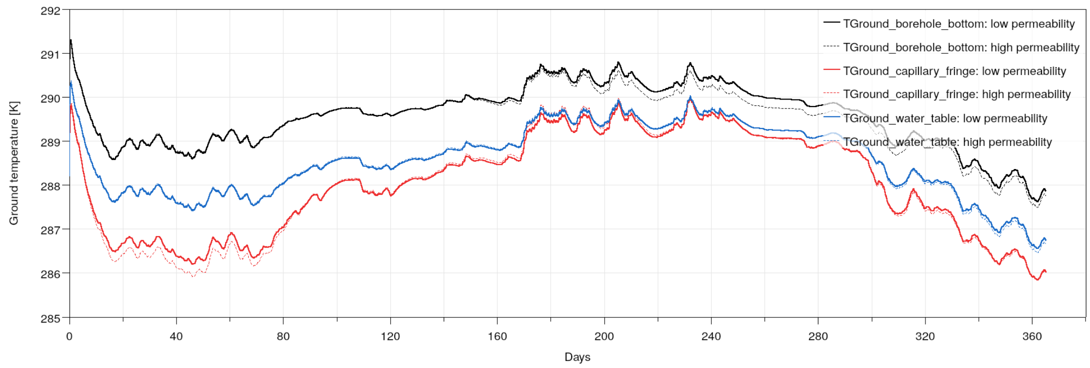


Figure 3: 2D constant-depth water-table case: temperature versus time at various depths, for low and high permeability cases

Figure 4 shows the temperature variation at various depths in the ground for the constant-depth and variable-depth water tables. When the ground bottom has sinusoidally varying pressure boundary, which produces a time-varying water table, the ground temperature at the borehole bottom shows larger fluctuation – a bit warmer in the first half of the year and cooler in the second half of the year. This is consistent with the pressure profile as shown in Figure 2. But for the ground temperature at the water-table depth, we cannot see a significant difference between the two pressure boundaries.

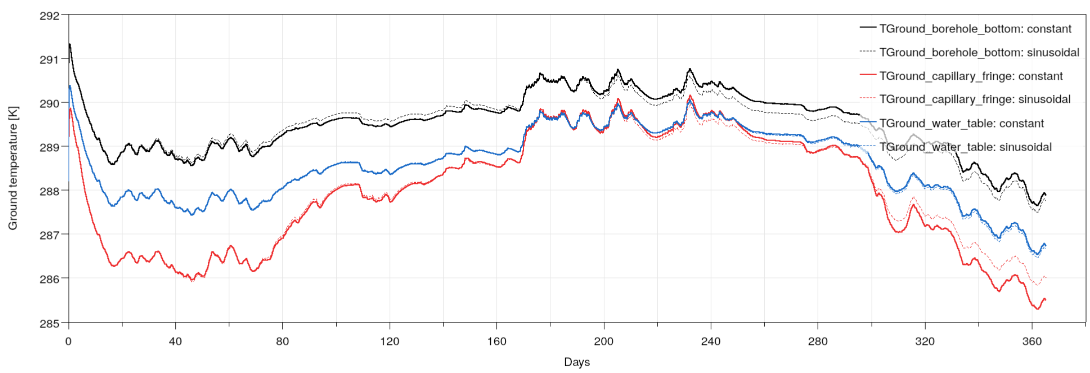


Figure 4: 2D deep water-table cases: temperature versus time at various depths, for constant water-table and time-varying water-table cases

4. 3D REGIONAL GROUNDWATER FLOW

Our previous cases, including the ones in Hu et al. (2020) and Doughty et al. (2021), did not consider regional groundwater flow. In this section, we look into the effect of groundwater flow, to investigate how significantly the water flow affects the heat transfer between the borehole and the ground. The next sections introduce the 3D ground simulation domain and boundary conditions that are required for simulating the regional water flow.

4.1 Grid

The 3D grid for the TOUGH simulation is shown in Figure 5. The y axis of the grid is aligned with the regional groundwater flow direction. By symmetry, in the x direction only one-half of the problem is included in the model. The simulation domain has x, y, z dimension 3 m x 21 m x 200 m. The 3-m x dimension represents one-half the distance between adjacent boreholes, in the direction perpendicular to regional groundwater flow. The 21-m y dimension is to allow for three boreholes spaced 6 m apart, with room for heat to be moved convectively with regional groundwater flow. The 200-m z dimension covers the 100-m long borehole, plus plenty of room for vertical conductive heat transfer. We consider just a single borehole, at x=0.125 m, y=11.88 m, z=-1 to -101 m.

Grid resolution is uniform laterally, with a grid size of 0.25 m. Vertically, the grid is finest near the ground surface (0.5 m thick grid blocks) to accurately represent surface heat exchange. The grid is also relatively fine in the vadose zone and at the water table at ~50 m depth (2.5 m thick grid blocks), to enable the capillary fringe to be accurately resolved. The maximum grid-block thickness of the borehole is 10 m, which matches the Modelica borehole grid resolution. When coupling with Modelica simulation in which the borehole is assumed to have 10 uniform sections, the Modelica calculated heat transfer rate that then becomes boundary for the TOUGH ground simulation is evenly distributed to the adjacent TOUGH grid. The TOUGH calculated borehole wall temperature that then becomes Modelica simulation boundary is averaged and then assigned to the adjacent Modelica grid.

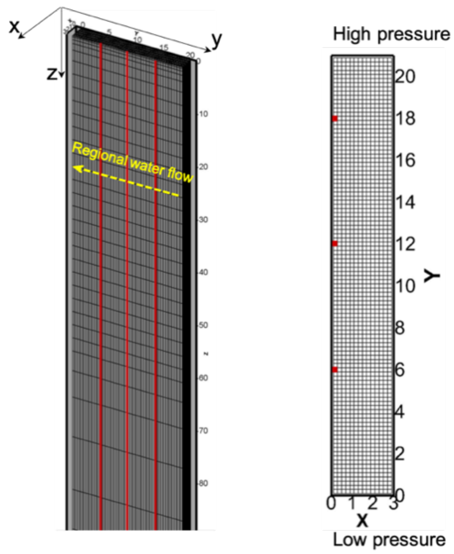


Figure 5: Perspective view (left) and plan view (right) of the 3D TOUGH grid. Red lines and dots show potential borehole locations. For the present simulations only one borehole at y ~ 12 m is considered.

4.2 Boundary and Initial Conditions

The top boundary of the model is the ground surface: the time-varying temperature is obtained from Modelica, whereas the pressure condition is held fixed at atmospheric pressure, with a relative humidity of 0.5. The bottom boundary of the model is closed to fluid and heat flow, but it is far enough away to not impact temperature conditions in the vicinity of the borehole. The lateral boundaries in the x direction are both closed to fluid and heat flow. The x = 0 boundary is closed because it is a symmetry line, and the x = 3 m boundary is closed to represent the existence of series of adjacent, identical boreholes separated by 6 m in the x direction. The lateral boundaries in the y direction are held at the same geothermal temperature profile and at different hydrostatic pressure profiles, which produces a hydraulic gradient from the upgradient boundary (y = 21 m) to the downgradient boundary (y = 0).

In order to create initial conditions for the Modelica/TOUGH simulation, a five-year TOUGH stand-alone simulation is run to allow the different hydrostatic pressure gradients imposed at the y boundaries of the model to produce equilibrated pressure, temperature, moisture, and regional groundwater flow distributions throughout the model. The magnitude of groundwater flow in response to the hydraulic gradient is uniform with depth below the water table, but decreases dramatically as water content decreases above the water table in the capillary fringe (Figure 6).

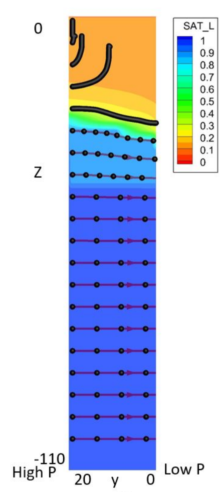


Figure 6: Initial conditions for the upper portion of the 3D Modelica/TOUGH simulation with regional groundwater flow. The water table is at about -50 m. The color field shows liquid saturation (water content), illustrating the hydraulic gradient from large to small y values. The black dots show equally-spaced timing markers on stream traces of regional groundwater flow. Where points are closer together, flow is slower.

4.3 Results

In Figure 7, the coupled simulation indicates that with regional groundwater flow, the water temperature out of the borehole is warmer in the heating season (winter) and cooler in the cooling season (summer). It reveals that in the heating season when heat is required from the above-ground energy system, more heat is transferred from the ground to the borehole. And in the cooling season when heat needs to dumped from the above-ground system, more heat is transferred from the borehole to the ground. This result is consistent with the heat transfer between the ground and the borehole (Figure 8), which shows a larger fluctuation when regional groundwater flow is considered. From the entire year's perspective, the occurrence of the regional groundwater flow causes more heat to be transferred from the borehole to the ground. All these results suggest that the regional groundwater flow causes stronger heat transfer between the ground and the borehole, due to stronger advective heat transfer. Figure 9 looks further into the groundwater flow's effect on the above-ground system, regarding the electrical consumption. In the figure, we see that there is no significant effect on the heat pump electrical consumption. This is because the pump control in the main district distribution loop compensates for the differences in loop temperatures, thereby causing the building service lines to have similar water temperatures among the cases. Thus, the heat pumps operate under the same condition. We therefore see more significant reduction on the pump electrical consumption, which is 6%. Overall, the total electrical consumption difference is 1.5%. However, the borehole outlet water temperature is preferable when considering regional groundwater flow, i.e., warmer in winter and cooler in summer. This suggests two optimization potentials: (a) the number of boreholes could likely be reduced, thereby saving capital costs and operational costs for pump energy for the borefield. (b) The lack of sensitivity of the compressor energy to the borefield temperatures suggests that the control was designed to be too conservative in favoring stability over performance. More aggressive control could make better use of the increased heat transfer. The main objective of the current control is to stabilize the district loop temperatures; relaxing this stability criteria could further improve the system efficiency beyond the results reported in Sommer (2020).

Figure 10 shows the results when the system operates for three years. It indicates that in the three years, there is no significant difference on the borehole outlet water temperature from year to year. The ground temperature profile is also consistent in the three years. Although we see that the profile of heat transferred from borehole to ground keeps ramping up, this in fact is an accumulation over the three-year period. The amount of heat transferred between them is the same each year.

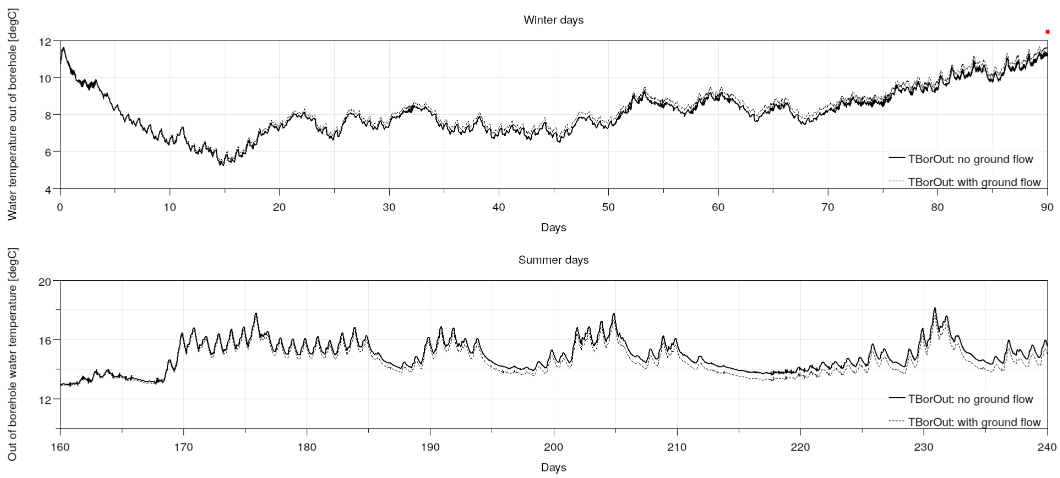


Figure 7: Borehole outlet water temperature in winter (upper figure) and summer (lower figure) days. Solid lines: no regional groundwater flow; dotted lines: with regional groundwater flow.

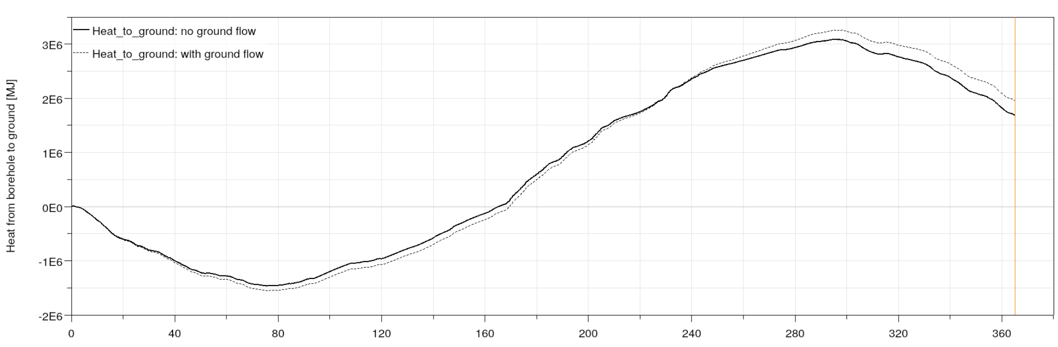


Figure 8: Heat transferred from borehole to ground. Solid line: no groundwater flow; dotted line: with groundwater flow.

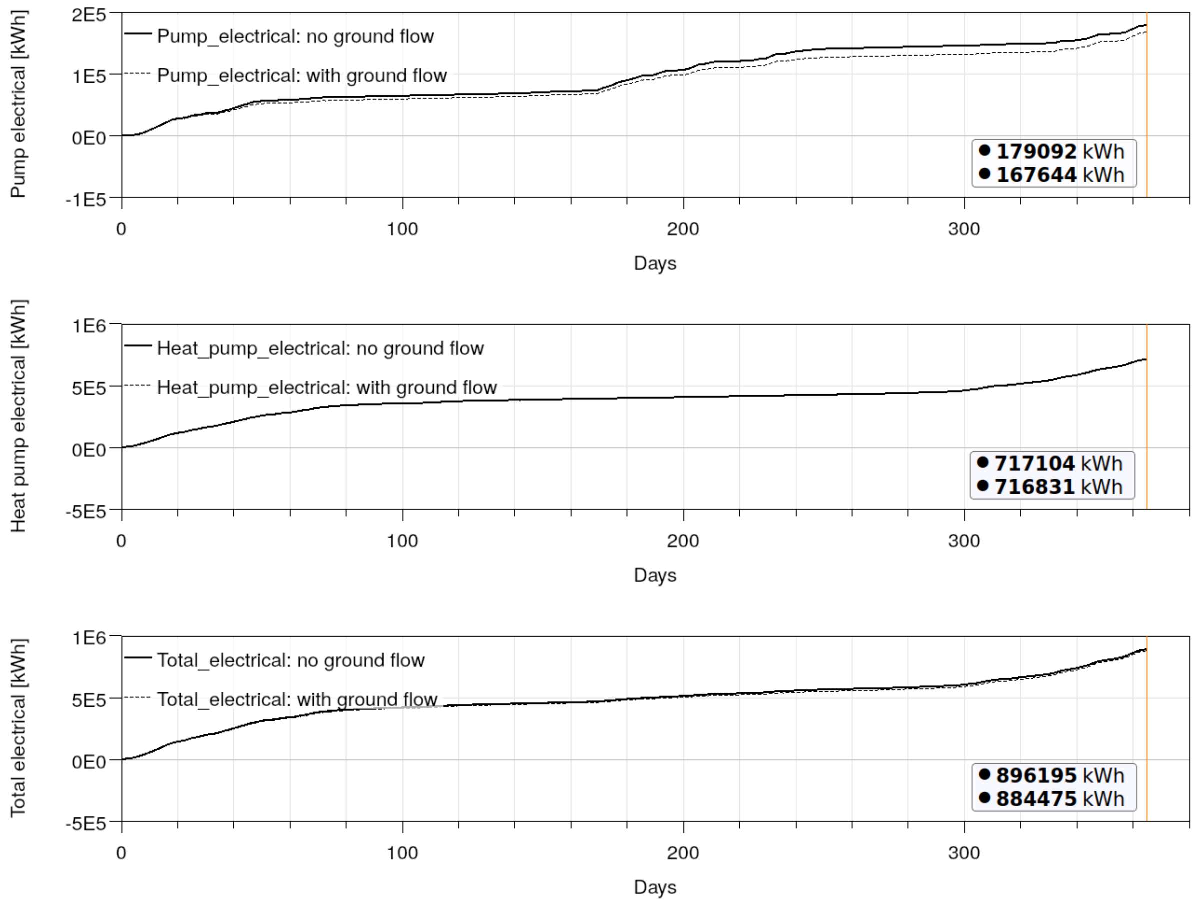


Figure 9: Pump, heat pump and total electrical consumption. Solid line: no groundwater flow; dotted line: with groundwater flow

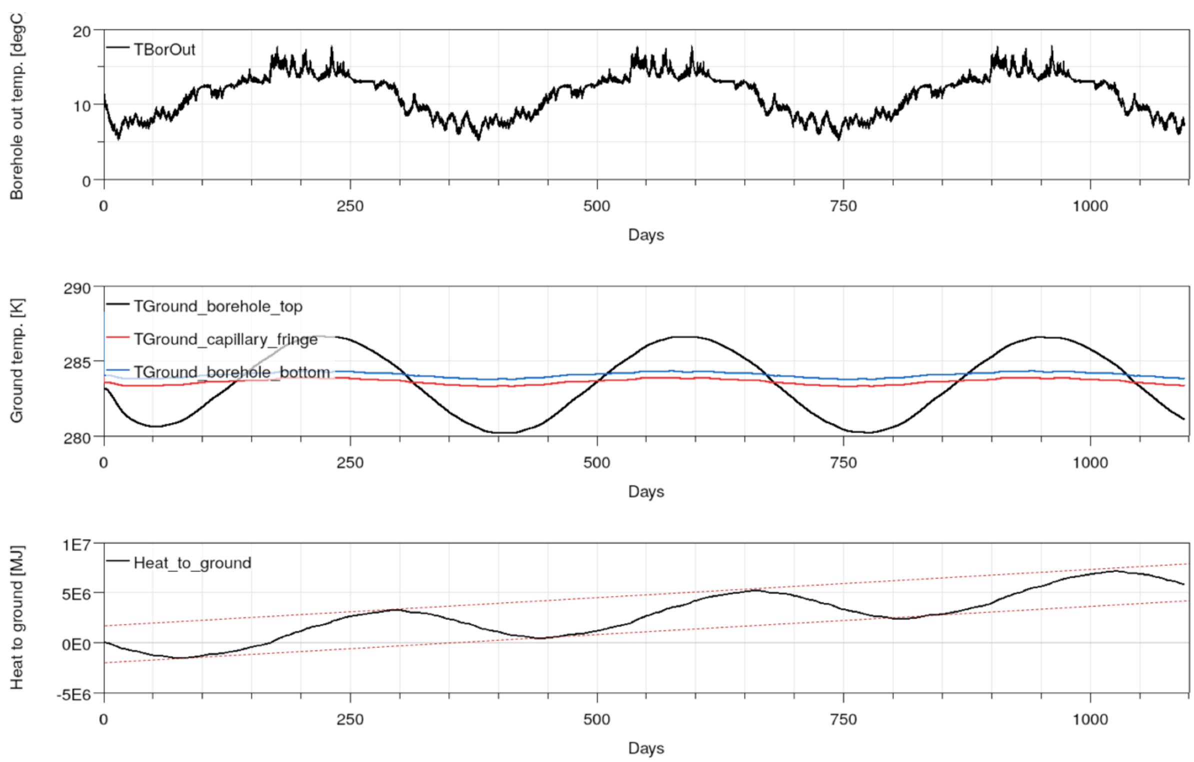


Figure 10: 3-year results: borehole outlet water temperature, ground temperature, and heat transferred from borehole to ground

5. CONCLUSIONS

We continue to develop the coupling between Modelica and TOUGH by considering more realistic subsurface scenarios than our previous studies (Hu et al., 2020; Doughty et al., 2021). We first considered the deep water-table cases in which the above-ground system is modelled with Modelica. It showed that when the ground has higher permeability, there will be more heat transfer between borehole and ground, which is consistent with natural convection in the groundwater enhancing heat transfer to and from the borehole. The variant bottom pressure (thus variant water table) causes larger ground temperature fluctuation but did not show significant effect on the overall heat transfer between the borehole and the ground. One possibility is that the water-table variations are just small perturbations above and below the constant water-table depth, so over the course of an entire year, differences in heat transfer near the water table balance out and the overall heat transfer is thus the same.

We also implemented 3D TOUGH simulations to study the effect of regional groundwater flow, with the assumption that the neighboring boreholes do not affect each other. The results showed that the groundwater flow can cause stronger heat transfer between the borehole and the ground due to the stronger advective heat transfer. More favorable borehole outlet water temperatures, warmer in winter and cooler in summer, are used by the above-ground district energy system. This then results in lower pump electrical consumption and reduced overall system operational cost. It demonstrates that without considering regional groundwater flow, such as in the g-function-based ground heat transfer simulation model, the design of the geothermal borefield for district energy system would be oversized and the calculation of the operation cost would not be correct. The results suggest that including the effect of ground water flow and improving the controls would allow a reduction in the number of boreholes under similar energy performance, thereby reducing capital and lifecycle costs.

Future work is still needed to consider more boreholes in the 3D ground simulation and to consider the interference between boreholes. It would also be necessary to consider different borehole/borefield geometries. Additionally, the coupling between Modelica and TOUGH could be improved, perhaps through the Function Mockup Unit (Modelica Association, 2021) interface, to provide a more efficient and robust coupling.

ACKNOWLEDGMENT

This material was based upon work supported by the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy (EERE), Geothermal Technologies Office, Low-Temperature Geothermal Program, under Award Number DE-AC02-05CH11231 with LBNL.

REFERENCES

Claesson, J. and Javed, S.: A Load-Aggregation Method to Calculate Extraction Temperatures of Borehole Heat Exchangers. ASHRAE Transactions 118(1), (2012), 530-539.

Doughty, C., Hu, J., Dobson, P., Nico, P., Wetter, M., Coupling subsurface and above-surface models for optimizing the design of borefields and district heating and cooling systems in the presence of varying water-table depth, Proceedings, 46th Workshop on Geothermal Reservoir Engineering, Stanford University, Stanford, CA (2021)

Hu, J., Doughty, C., Dobson, P., Nico, P., Wetter, M., Coupling Subsurface and Above-Surface Models for Design of Borefields and Geothermal District Heating and Cooling Systems, Proceedings, 45th Workshop on Geothermal Reservoir Engineering, Stanford University, Stanford, CA (2020).

Jung, Y., Pau, G., Finsterle, S., and Doughty, C.: TOUGH3 User's Guide, Version 1.0, *Report LBNL-2001093*, Lawrence Berkeley National Laboratory, Berkeley, CA (2018).

Modelica Association: Functional Mock-up Interface for Model Exchange and Co-Simulation, Version 2.0.3, 2021

Picard, D. and Helsen, L.: Advanced Hybrid Model for Borefield Heat Exchanger Performance Evaluation: An Implementation in Modelica, Proceedings, the 10th International Modelica Conference, p. 857-866. Lund, Sweden. March 2014.

Pruess, K., Oldenburg, C., and Moridis, G.: TOUGH2 User's Guide, Version 2.1, *Report LBNL-43134*, Lawrence Berkeley National Laboratory, Berkeley, CA (2012).

Sommer, T., Sulzer, M., Wetter, M., Sotnikov, A., Mennel, S., and Stettler, C.: The reservoir network: A new network topology for district heating and cooling. Energy, 199, 2020, doi: 10.1016/j.energy.2020.117418.

van Genuchten, M.Th.: A closed form equation for predicting the hydraulic conductivity of unsaturated soils, Soil Sci. Soc. Am. J., 44, (1980), 892–898.

Wetter, M., Zuo, W., Nouidui, T.S., and Pang, X.: Modelica Buildings Library, J. Building Performance Simulation, 7, (2014), 253–270.

Xu, T., Sonnenthal, E., Spycher, N., and Zheng, L.: TOUGHREACT V3.0-OMP Reference Manual: A Parallel Simulation Program for Non-Isothermal Multiphase Geochemical Reactive Transport, *Report LBNL-DRAFT*, Lawrence Berkeley National Laboratory, Berkeley, Calif., (2014).