# Coupling Subsurface and Above-Surface Models for Design of Borefields and Geothermal District Heating and Cooling Systems

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## ABSTRACT

Dynamic energy simulation is important for the design and sizing of district heating and cooling systems with geothermal energy storage in borefields. Current modeling approaches in building and district energy simulation tools typically consider heat conduction through the ground between boreholes, without flow of groundwater. On the other hand, detailed simulation tools for subsurface heat and mass transfer exist, but these fall short in simulating building and district energy systems. To support the design and operation of such systems, this study presents a model coupling between a software package for building and district energy simulation, and software for detailed heat and mass transfer in the ground. For the first, we use the free 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 simulators, which were initially designed for geothermal reservoir engineering and also have been used extensively for aquifer and borehole thermal energy storage. The current version of TOUGH 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. This paper describes the design of the coupling of these software packages, and how the time-dependent boundary conditions for the borehole walls are synchronized for use in Modelica and TOUGH. It also presents the validation of the coupled modeling and closes with the discussion of further model improvements.

#### 1. INTRODUCTION

Geothermal resources are considered a clean and sustainable form of renewable energy and have been applied as the heating and cooling source 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, a dynamic model of the borefield and DHC system that can consider subsurface fluid flow and be coupled to existing simulation models for DHC systems and building loads is still a challenge to be addressed.

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 ground water 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, which greatly impacts 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.

This paper presents a modeling approach to couple the above-surface district energy system modeling with Modelica and subsurface ground response modeling with TOUGH. It starts with the introduction of the coupling approach and then shows the results of validating the coupling approach. We end this paper by introducing next steps to improve the coupled modeling.

## 2. MODELICA AND TOUGH COUPLING APPROACH

This study focuses on a district heating and cooling system that 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 can be divided into multiple segments.
- Each borehole has multiple segments (N) and each segment has a uniform temperature.
- Initial ground temperature has a profile as shown in Figure 1c.

Based on these assumptions, all boreholes within the borefield behave identically, so only one need be modeled.

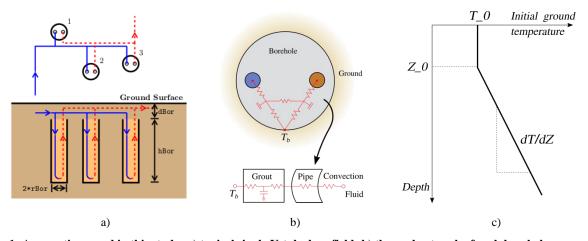


Figure 1: Assumptions used in this study: a) typical single U-tube borefield; b) thermal network of each borehole segment; c) initial ground temperature

Table 1: Parameters and the values used for the borefield

Parameters	Value	Description
hBor	100 m	Height of the borehole
N	10	Number of borehole segments
rBor	0.075	Borehole radius
dBor	1.0 m	Borehole buried depth
DBor	6.0 m	Distance between boreholes
dT/dZ	0.01	Vertical temperature gradient of undisturbed soil
T_0	283.15	Initial ground temperature from which ground gradient starts
Z_0	10 m	Depth below which ground temperature gradient starts

## 2.1 Coupling interface

The class Buildings.Utilities.IO.Python27.Real\_Real in the Modelica Buildings Library is used as the interface to integrate the TOUGH and Modelica simulations. This class can send data to Python functions, and obtain data from Python functions. For example, it allows use of Python to communicate with web services and with hardware, or as in this study, to do other computations inside a Python module that calls an external simulator like TOUGH. Through the interface (Figure 2), the coupled simulation, which primarily runs in the

Modelica environment, calls the module *doStep* (Figure 3) of the Python function *GroundResponse*. The interface also specifies the number of values that are read from (*nDblRea*) and written to (*nDblWri*) the Python function; sample period (*samplePeriod*), which defines how often Modelica should call the Python function; flag (*flag*) that specifies the type of values (current value, average over interval, or integral over interval) written to the Python function; and check (*passPythonObject*) if the Python function needs to pass Python objects between one invocation to another.

```
1 Buildings.Utilities.IO.Python27.Real_Real pyt(
2    moduleName="GroundResponse",
3    functionName="doStep",
4    nDblRea=nSeg,
5    nDblWri=2*nSeg+1,
6    samplePeriod=samplePeriod,
7    flag=flag,
8    passPythonObject=true);
```

Figure 2: Instantiation of the Modelica Python interface to call for TOUGH simulator

```
def doStep(dblInp, state):
 1
 2
      # retrieve state of last invoke
      {tLast, Q, T} = state['tLast'], state['Q'], state['T']}
 3
      # update TOUGH input files for each TOUGH call
 4
      os.system("./writeincon < writeincon.inp")
 5
      # conduct one step TOUGH simulation
      os.system("/.../tough3-install/bin/tough3-eos1")
 7
      # extract borehole wall temperature for Modelica simulation
 8
 9
      os.system("./readsave < readsave.inp > out.txt")
      T = borehole temperature('out.txt')
10
      # update state
      state = {'tLast': tim, 'Q': Q, 'T': T}
12
13 return [T, state]
```

Figure 3: Pseudo code of Python module that conducts TOUGH simulation

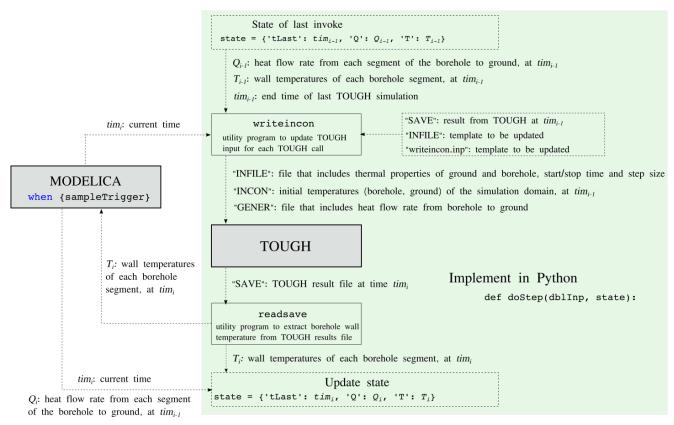


Figure 4: Workflow for coupling Modelica and TOUGH simulation through Python interface 2.2 Coupling framework

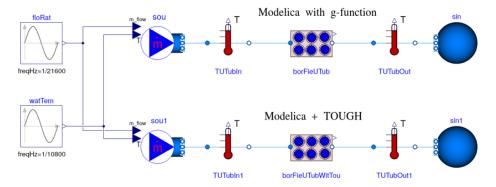
Figure 4 shows the coupling framework. When the Modelica variable *sampleTrigger* is *true*, Modelica calls a Python module that invokes TOUGH. This Python module has, as an input/output argument, an object called state that contains the synchronization time instant, the

heat flow rates from the ground and the temperatures of each borehole segment. In the first invocation of Python, this object is not yet initialized. Python therefore takes the initial ground temperature from Modelica, and initializes this object. It then writes the TOUGH input files, invokes TOUGH and reads the TOUGH output files to obtain the new borehole temperatures. During this synchronization time step, TOUGH advances by a fixed synchronization time step, holding the borehole-to-ground heat flow rate Q constant. After TOUGH completed, Python reads the new borehole segments temperature T and returns it to Modelica. Python also stores the new borehole temperatures in state for use in the next call.

## 3. RESULTS VALIDATION

The coupled modeling approach was validated by comparing its simulation results with results calculated by a model based on g-function. For the validation, the TOUGH simulation disabled groundwater flow so the heat transfer in the ground is purely by conduction, which is the same as the g-function-based model. Two models were created for the validation, i.e., a pure-ground-response model and a closed-loop district energy system model. The pure-ground-response model, as shown in Figure 5a, ensures that the same amount of water with the same temperature comes into both g-function-based and TOUGH-based borefields. The coupled model was then validated through the closed-loop simulation of a district energy system. Besides a sewage heat exchange station, the district energy system (Figure 6) also includes a 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, commit a2667c0. The needed files for TOUGH simulation and the coupling interface are in folder Buildings/Resources/Python-Sources.

The pure ground-response simulation results shown in Figure 5b indicate that the TOUGH-based borefield can capture the same ground response as the one from the g-function-based borefield. The borefield outlet water temperatures from these two models match well, with the average difference of 0.28 Kelvin.



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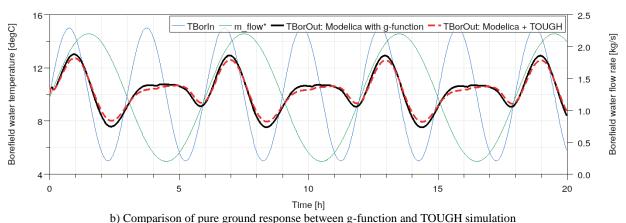


Figure 5: Pure ground response model and the simulation results with both models

With the same borehole configuration, we conducted annual closed-loop district energy system simulations with both borefield models. Figure 7 shows the borehole wall temperature and heat flow rate between borehole and ground, which are the coupling variables between Modelica and TOUGH. We can see the good agreement between the coupled Modelica + TOUGH simulation and the purely Modelica simulation. However, the coupled simulation, which has the sample period of 3600 seconds in this test, required 1390 seconds to finish and it is slower than the 1160 seconds of pure Modelica simulation. One reason of the slow computing time is due to the file I/O and by starting a new TOUGH process at each synchronization step. This will be addressed in our future developments when using the Functional Mockup Interface standard (Blochwitz et al., 2012).

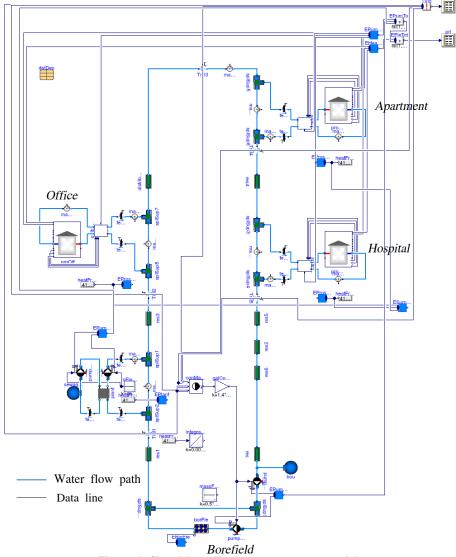


Figure 6: Closed-loop district energy system model: Buildings.Examples.DistrictReservoirNetworks.Examples.Reservoir3Variable\_TOUGH

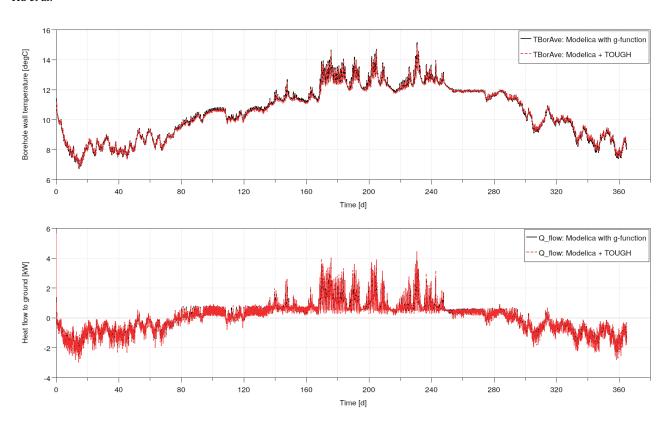
# 4. DISCUSSION AND FUTURE WORK

This paper presents our first demonstration of coupling subsurface TOUGH simulation and above-surface Modelica simulation for design of a borefield and district heating and cooling system. The coupled model was validated by a g-function based Modelica model, by running a pure ground-response simulation and a closed-loop district energy system simulation. The good agreement between the simulation results with these modeling approaches, for the case in which heat transfer underground is purely by heat conduction, illustrated that the Modelica + TOUGH coupled model can capture the dynamics of the closed-loop system, from ground response to building load changes. However, more work is needed to further improve the coupling model as presented below:

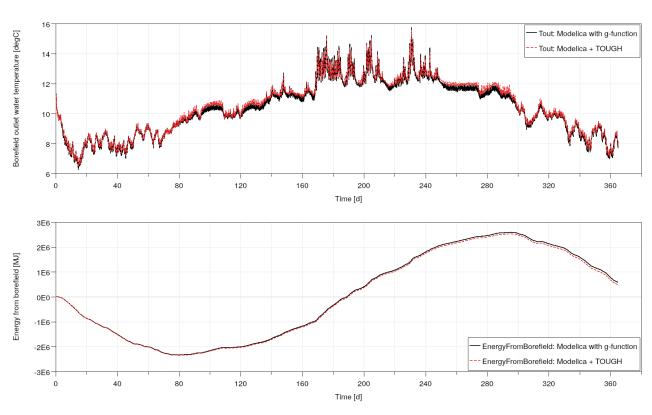
- 1) Adaptive sampling period to avoid temperature pulses.
- 2) Streamline the configuration of the coupled models:
  - a) Through the Modelica Python interface to generate the mesh file for the TOUGH simulation.
  - b) Make the ground properties parameters in Modelica and write them to TOUGH input files through Python interface.
  - c) Encapsulate the TOUGH model as a Functional Mockup Unit (Blochwitz et al., 2012).
- 3) Enable groundwater flow in TOUGH simulation and investigate fluid flow effects on the system design, both borefield and district energy system designs.

## ACKNOWLEDGEMENT

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a) Borehole wall average temperature and heat flow rate from one borehole to ground



b) Borefield outlet water temperature and the energy extracted from the ground

Figure 7: Closed-loop district energy system simulation results with both models

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