Supplement of

City-scale heating and cooling with Aquifer Thermal Energy Storage (ATES)

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S1 Numerical subsurface model of Freiburg

The numerical 3D finite element flow and heat transport subsurface model of the study area serves as a baseline to evaluate the representativeness of the box models regarding ATES power density in the city of Freiburg. The exact delineation of the study area is done in a way so that the majority of the built-up area of Freiburg is included and considers the hydraulic and topographic conditions. The model covers an area of about 72 km^2 and includes the Dreisam valley in the southeastern part and a large portion of the Dreisam alluvial cone in the northwest. The southeastern boundaries are defined based on the topographic transition from the Upper Rhine Graben to the Black Forest. This is also reflected in the 2nd kind constant-flux boundary conditions (BCs) set at these boundaries (Fig. S1.1) which represent the inflow into the study area from the adjacent Black Forest. The remaining model boundaries in the southeast as well as the northwestern boundary of the study area correspond to hydraulic head contour lines (Fig. 1) and accordingly feature 1st kind constant-head BCs. The southwestern as well as the northeastern boundaries are set up perpendicular to the groundwater hydraulic head contour lines. The Dreisam River flowing through the study area is implemented as a 3rd kind head-dependent flux BC with a flow rate dependent on the Dreisam water level in order to account for the gaining steam regime present in the study area (Villinger, 1999). A 2nd kind no-heat flux BC is applied on the top surface of the Freiburg model. This approach of thermally insulating the top surface and thus impeding any exchange of thermal energy with the atmosphere is consistent with the box models and results in larger thermal plumes and thus in more conservative power density estimations (Ohmer et al., 2022).

The Freiburg model consists of two layers representing the Neuenburg Formation and the Breisgau Formation. The bottom of the model is formed by the base of the Breisgau Formation (data from Wirsing and Luz, 2005), whereas the model's top side is created from the digital elevation model shown in Fig. 1. According to Villinger (1999) and as shown in Fig. 1c, the Neuenburg Formation is covered by a thin loess layer of mostly less than 1 m thickness in some parts of the study area. However, this layer is not implemented in the Freiburg subsurface model due to its location above the saturated zone in most parts of the area. The hydraulic and thermal parameters used in the model are listed in Table 1.

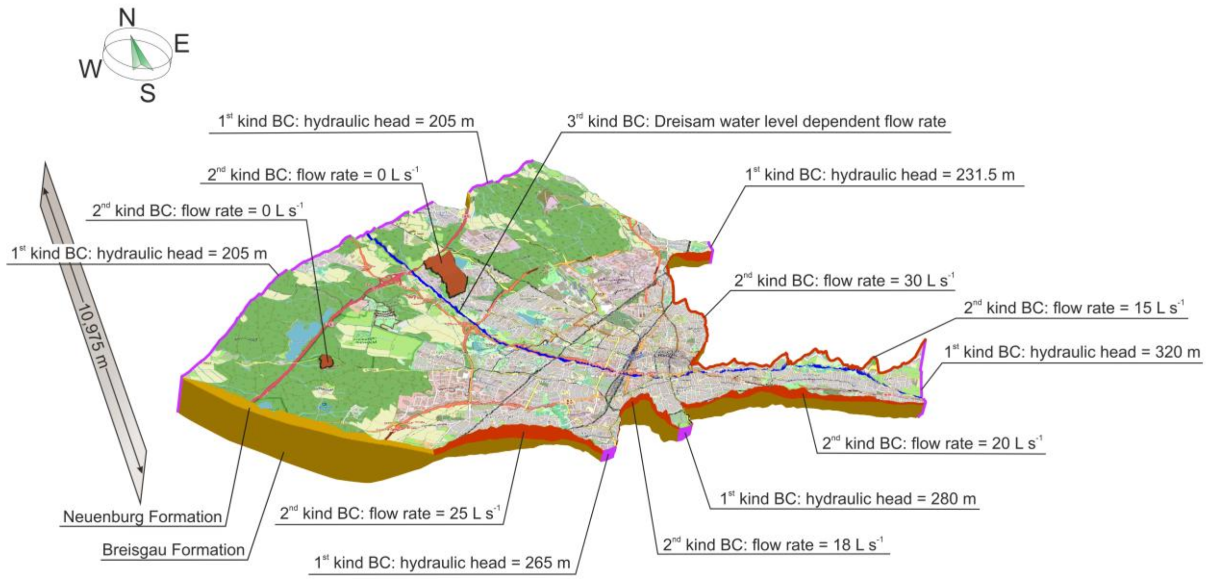

Figure S1.1. Numerical subsurface model of Freiburg consisting of the Neuenburg Formation (upper layer) and the Breisgau Formation (lower layer). The model illustration is ten times stretched in vertical direction. © OpenStreetMap contributors 2022. Distributed under the Open Data Commons Open Database License (ODbL) v1.0.

In order to achieve a hydraulic head distribution in the Freiburg model best fitting to the hydraulic head contour lines shown in Fig. 1, the stationary flow model is calibrated using the hydraulic conductivity of the Neuenburg Formation. Starting from the initial hydraulic conductivity distribution given by Wirsing and Luz (2005), the calibration is done using existing hydraulic head measurement data across the study area. Fig. S1.2 shows the calibration results. The coefficient of determination of 0.998 and a root mean square deviation of 1.21 m indicate a high capability of the model to reproduce the hydraulic head measurements.

Based on the calibrated stationary flow model, a transient subsurface flow and heat transfer model is created with implemented ATES systems in either the Neuenburg or the Breisgau Formation. Using the areal extents of the thermally affected zones (TAZ) around individual ATES systems as determined from the box models allows a systematical ATES placement in the Freiburg subsurface model. The final model consists of about 1.5 million tetrahedral elements. This number increases during the modeling runtime due to the utilization of the adaptive mesh refinement option implemented in COMSOL Multiphysics. The modeling results are shown in section 3.5, Fig. 11 of the main manuscript and discussed regarding the box models' representativeness.

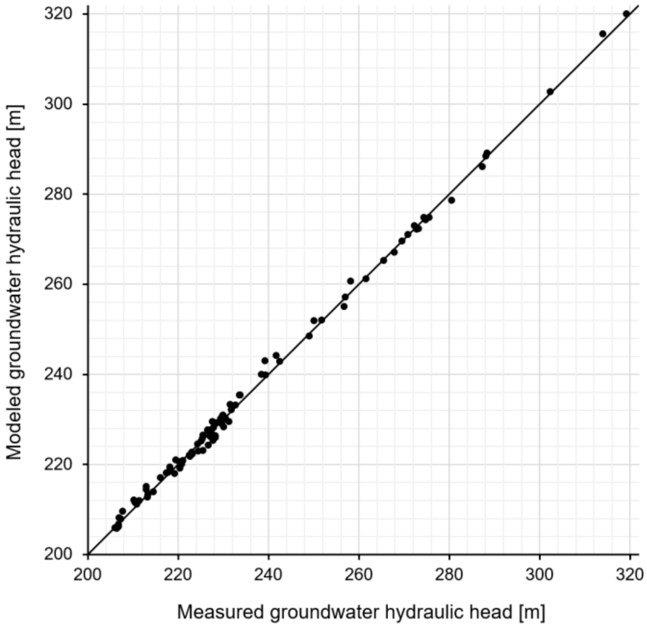

Figure S1.2. Modeled groundwater hydraulic heads plotted against measured groundwater hydraulic heads. The calibration results in a high coefficient of determination of 0.998. The root mean square deviation is 1.21 m.

S2 Power density results when using the ± 1 K-isotherms

Contrary to many previous publications on the topic of thermal plume propagation in the subsurface, we use the ± 0.5 K-isotherms from the box models to delineate the TAZ and calculate the power densities. However, as an additional information, Fig. S2 shows the power density values calculated from the TAZ as defined by the ± 1 K-isotherms after 30 years of ATES operation. On average, these values are about 2.1 times as high as the power densities shown in Fig. 8.

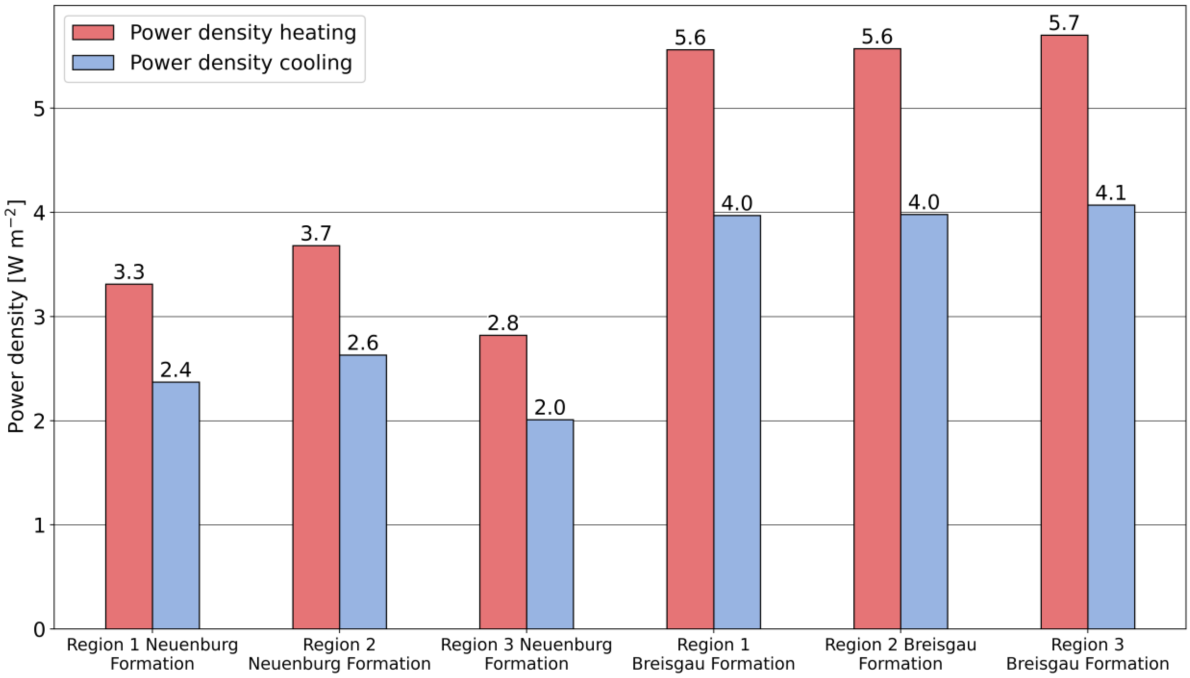

Figure S2. ATES Power densities for Neuenburg and Breisgau Formations when using the ± 1 K-isotherms after 30 years for delineating the TAZ. ATES systems in the Neuenburg Formation are modeled as 2-doublet configurations. Systems in the Breisgau Formation use a 3-doublet configuration.

S3 Heating energy mix in Freiburg

Table S3 provides information about the final energy mix for space and water heating in the city of Freiburg for the year 2020.

Table S3. Final energy mix for space and water heating in Freiburg in 2020 with the respective emission factors for each energy source. Data from GEF Ingenieur AG et al. (2021).

Energy source	Final energy mix for space and water heating [%]	Emission factor [$tCO_2eq\ MWh^-$
Natural Gas	54	0.247
District heating	22	0.193[a]
Heating oil	17	0.318
Biomass	6	0.025
Heat pumps	1	0.118[b]
ATES	0	0.083[c]

[a] Freiburg mix.
[b] Calculated using seasonal COP = 3.5 and electricity emission factor of 0.412 $tCO_2eq\ MWh_{el}^{-1}$.
[c] Stemmle et al. (2021).

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