

# ***OPTIMIZATION OF AN ENERGY SYSTEM MODEL COUPLED WITH A NUMERICAL HYDROTHERMAL GROUNDWATER SIMULATION***

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## **Overview**

To achieve a climate neutral society in the future, all energy sectors will have to change significantly. This primarily involves replacing fossil fuels with renewable resources. Residential heating and cooling is a sector with significant potential for reducing CO<sub>2</sub> emissions. One of the promising technologies in this sector, among other types of heat pumps, are groundwater heat pumps (GWHPs). GWHPs use the thermal energy of groundwater and generally offer a higher efficiency than other types of heat pumps. In heating mode, these systems extract heat from an aquifer and thus lower the groundwater temperature. This results in thermal anomalies (thermal plumes) in the aquifer that propagate downstream in the groundwater flow direction and can reach neighboring systems. If the downstream systems also work in heating mode, such interactions will reduce their efficiency, since the efficiency of GWHPs depends significantly on the groundwater temperature at their extraction wells. Therefore, regulations follow the first-come first-serve principle and protect existing systems from negative interactions by new systems. These regulations must be taken into account when analyzing future energy systems with a high share of GWHPs, as the thermal potential of the resource groundwater is limited.

In general, energy system optimization models (ESOMs) are used to estimate the optimal energy system transitions towards future CO<sub>2</sub> reduction targets, i.e. to find optimal technology mixes in future energy systems. On the other hand, a hydrothermal numerical groundwater simulation model is required to quantify the thermal groundwater potential of a specific area. Therefore, in order to integrate the thermal groundwater potential into ESOMs, it is necessary to couple both models. Such a coupling scheme is developed within the research project GEO.KW [1] based on the open-source software frameworks (1) urbs [2] that is used to define, solve and analyze the underlying ESOM, which in this case is the model of a residential heating sector. urbs is a linear programming framework that relies on the multiple-input-multiple-output representation of different processes in ESOMs, such as different power generation units, energy storages, or transmission lines; (2) PFLOTTRAN [3] that is used for numerical simulation of groundwater flow and heat transport based on the finite volume method and (3) preCICE [4] a coupling library that can efficiently couple different simulations/solvers. The present study focuses on the optimization part within the coupling and introduces the new optimization approach developed for the overall coupling scheme.

## **Methods**

The underlying optimization problem is a black-box optimization, where the groundwater simulation represents the black box constraints. Evaluating these constraints is computationally intensive as the groundwater simulations are high fidelity numerical simulations applied to a 3D domain representing various subsurface geological layers including the aquifer. Using the common derivative-free global optimization methods for solving black-box problems, such as evolutionary algorithms, is not feasible in this case because they require a large number of constraint evaluations. Therefore, a new optimization approach is presented in this study, which requires a relatively small number of black box evaluations, i.e. groundwater simulations. In addition to the computationally intensive groundwater simulations, the spatially embedded ESOM is also computationally intensive due to the large size of the problem (large number of optimization variables and constraints), since each individual building is modeled and no spatial aggregation is carried out. The proposed optimization method addresses this problem in the sense that the original ESOM area is decomposed into smaller regions, which are then individually optimized, i.e. considered as separate smaller ESOMs. These optimization regions are naturally connected by the regional groundwater flow. This means that a GWHP system installed in an upstream region will change the groundwater temperature only in the downstream direction and therefore, may only affect downstream systems located in its own ESOM or a downstream ESOM. Thus, the entire area is separated into optimization regions based on the groundwater conditions, i.e. the thermal plumes of all potential GWHPs, which were calculated using simplified analytical

formulas and the estimated heating demands for all buildings. To decompose the original area into smaller regions, a new decomposition method is proposed that first uses constrained k-means clustering with background knowledge to define clusters throughout the domain, and then combines the resulting clusters to obtain the final optimization regions (ESOMs).

Once the optimization regions are defined, the entire optimization procedure of the ESOMs coupled with the groundwater simulation is carried out iteratively. This means that in one iteration half of the optimization regions (ESOMs) are activated (optimization is performed) and a maximum of one new GWHP per region is selected for installation. After that, the groundwater simulation is performed and the resulting groundwater temperatures are used to check if all regulatory conditions are met and to update the efficiency of GWHPs. If all regulatory conditions are met for the selected GWHP, that system will be installed and otherwise removed from the list of potential systems. Finally, the next optimization iteration is started, i.e. the other half of the optimization regions are activated and the previous procedure continues with adding/removing one of the potential GWHP systems per region. The selection of potential GWHPs to install/remove in each iteration is done using standard linear programming in each individual ESOM (optimization region) and the Gurobi optimization solver. The whole optimization procedure (coupled simulation) ends as soon as there are no more potential GWHPs left or if none of the ESOMs selects new GWHPs (e.g. if a more optimal technology is available in the technology mix).

## Results

The proposed optimization method is tested on a real case study in the city of Munich, Germany. The study case consists of 1897 buildings and has a total area of approximately 740 ha. To demonstrate the validity of the method, two optimization scenarios are considered: the maximum expansion of GWHPs with the current and the future (year 2050) climate situation and the building stock. The results show that the proposed methodology successfully determines the optimal installation (placement) of GWHPs where all regulatory conditions are met and therefore, the spatial potential of thermal groundwater use is maximized. The decomposition of the area resulted in 26 optimization regions, which in the end are relatively evenly populated with new GWHP systems. This decomposition also enabled the parallelization of the ESOMs, since they can be solved independently at the same time in each coupling iteration. Furthermore, the comparison of the results of the two optimization scenarios shows that the proposed optimization procedure and the corresponding coupling scheme are able to correctly consider the possible future environmental (groundwater) impacts and the building stock changes.

## Conclusions

The present study introduces a new approach to optimize energy system models coupled with numerical hydrothermal groundwater simulations. Such coupling schemes are required to analyze future energy systems with a high penetration of GWHPs, since GWHP efficiency and installation approvals depend significantly on groundwater temperatures. The proposed optimization approach combines different strategies to solve the underlying black-box optimization problem. These strategies include iteratively adding or removing the potentially new GWHPs, which significantly reduces the number of required groundwater simulations within the coupling, as well as decomposition procedures that split the original ESOM into smaller independent ESOMs, which are then solved in parallel. The approach is successfully tested with a real case study in which the spatial groundwater thermal potential is maximized.

## References

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