Geothermics 95 (2021) 102132

Contents lists available at ScienceDirect

Geothermics

journal homepage: www.elsevier.com/locate/geothermics

Machine learning enhancement of thermal response tests for geothermal potential evaluations at site and regional scales

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ARTICLE INFO

Keywords:
Geothermal energy
Machine learning
Thermal response testing
Borehole heat exchangers
Data-driven predictions

ABSTRACT

This study explores and validates a machine learning approach for the practical, effective, and precise prediction of the thermo-physical characteristics that are essential for the analysis and design of shallow geothermal systems, including borehole heat exchangers: (i) undisturbed ground temperature, (ii) ground effective thermal conductivity, and (iii) borehole thermal resistance. Benefiting from 174 thermal response tests from central and western Switzerland, the algorithm is used to provide accurate site-specific as well as regional-scale predictions of the investigated thermo-physical characteristics, which in turn can serve preliminary yet representative evaluations of the geothermal potential of even very broad areas.

1. Introduction

Buildings represent the largest energy-consuming sector in developed countries: while accounting for over one-third of the global final energy consumption associated with domestic hot water production, space heating, and space cooling, they represent a major source of carbon dioxide emissions (Organisation de coopération et de développement économiques, 2013). Decreasing the environmental impact of buildings via technologies that harvest renewable energy sources is a crucial challenge for the sustainability of human activity. In this context, employing ground source heat pump (GSHP) systems that use the natural quasi-constant temperature of the subsurface to provide renewable energy to the built environment represents one of the most promising sustainable solutions available (Rybach and Mongillo, 2006; Saner et al., 2010). Among the various types of GSHP systems that can be used for this purpose, vertical borehole heat exchangers (BHE) represent an attractive technology due to their high efficiency and minimal interference with the landscape (Lund et al., 2004). In view of these advantages, BHE applications are tremendously growing worldwide, particularly in Switzerland, which currently is the country with the highest number of installations per square metre of land across the world (for example, the year 2019 was characterised by 1'915 MW of installed heating power) (Suisse Energie, La géothermie, 2020) .

The thermo-physical characterisation of the shallow underground (e.g., down to 400 m) is a prerequisite for the design of GSHP systems, including BHEs and other shallow geothermal heat exchangers. This characterisation is typically considered with varying levels of accuracy depending on the size of the geothermal installation. In general, the design of small installations (individual BHEs serving small houses) is based on the use of design charts and recommendations that include some information about the subsurface characteristics, as well as a safety factor that yields a greater probe length to account for uncertainties in the subsurface characteristics (e.g., local geological or hydrological properties). For larger installations (BHE groups and fields serving buildings and industrial facilities), accurate and site-specific characterisations of the underground through field testing are carried out to limit the approximations and the likely higher drilling costs involved with the previous design method (proportional to the probe field oversizing).

Currently, the determination of the design parameters for relatively large shallow geothermal applications mainly resorts to in situ thermal response tests (TRT), which involve the application of a known thermal load to a representative BHE and the measurement of the resulting changes in temperature of the fluid circulating in the heat exchanger pipes. Through such tests, three key design parameters can be determined: (i) the undisturbed ground temperature, (ii) the ground effective thermal conductivity, and (iii) the borehole thermal resistance. Therefore, TRTs represent a powerful source of information for the design of geothermal heat exchangers because they provide estimates of physical parameters that account for the local hydrogeological and thermo-

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https://doi.org/10.1016/j.geothermics.2021.102132
Received 13 November 2020; Received in revised form 5 April 2021; Accepted 28 April 2021
Available online 19 May 2021
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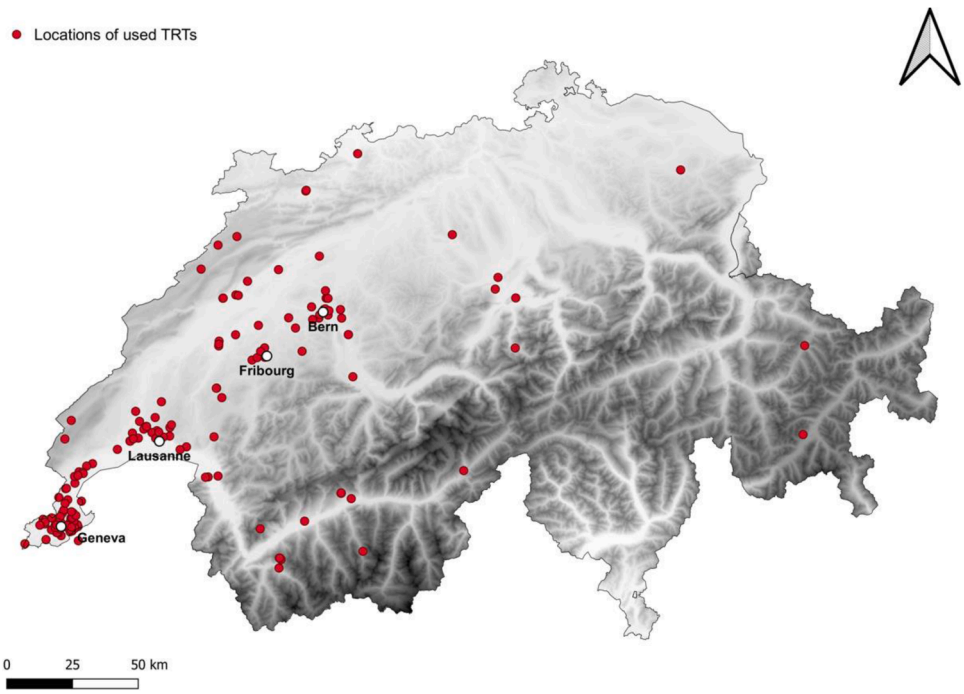

Fig. 1. Spatial distribution of the collected TRT reports across Switzerland (over a Digital Elevation Model of Switzerland).

physical characteristics encountered at any given site. These characteristics are inherently *embedded* in the temperature data measured through TRTs, as they depend on the local subsurface characteristics: for instance, interpretation of the temperature data recorded through TRTs will always provide a higher estimate of effective thermal conductivity for a saturated soil than the same soil under dry conditions, while a lower estimate as compared to the same soil under the influence of groundwater flow. Therefore, if one could establish a link between the features of borehole logs and past corresponding TRT results, it would be theoretically possible to achieve the following: (1) determine the design parameters targeted by TRTs for all sites where subsurface characteristics are known through borehole logs and TRTs are unavailable, or (2) characterise the local subsurface characteristics of any site where TRT results are accessible and borehole logs are scarce or unavailable.

In this framework, scientific machine learning offers a unique opportunity to account for multiple explanatory variables (commonly called features in machine learning applications) based on past testing experience, facilitating the consideration of both fundamental physical phenomena and local singularities with sufficient data. In recent years, increasing applications of machine learning have explored the design of geothermal systems. Some investigations have focused on the prediction of the energy performance of geothermal applications (Makasis et al., 2018), while others the use of TRT data to develop geothermal potential maps (Assouline et al., 2019; Kalogirou et al., 2015, 2012), via rather widely used algorithms, such as artificial neural networks and random forest. According to Zhou et al. (2019), while various models have been applied, their scope of application could be strengthened by using broader experimental datasets, instead of the customary small experimental platform and/or numerical simulation data used for such purpose. In particular, reference to real-world data, while representing a challenge in terms of information pooling and uniformization, represents a significant opportunity to enhance current analyses and design capabilities.

This paper significantly broadens the scope of existing studies that employ machine learning methods to address the analysis and design of geothermal systems. Specifically, by exploring and validating an innovative boosting algorithm trained on in situ TRT data that derive from 174 boreholes at the regional scale in central and western Switzerland, this study addresses the data-driven assessment of crucial thermo-physical characteristics for the analysis and design of BHEs: (i) the undisturbed ground temperature, (ii) the ground effective thermal conductivity, and (iii) the borehole thermal resistance. This endeavour is tackled through two series of predictions: site-specific predictions aiming at estimating thermo-physical characteristics (i-iii) for local geothermal applications; regional-scale predictions aiming at determining thermo-physical characteristics (i-ii) for regional and national feasibility studies and planning. The results of site-specific predictions are compared with actual borehole data, while those of regional-scale predictions with a Geographical Information System (GIS) database currently provided by administrative authorities.

In the following, the machine learning method is first presented with reference to the employed model algorithm and data. Next, the results for the site-specific prediction and the regional-scale mapping are presented, analysed, and compared to the accuracies expected in practice. Then, a discussion is presented. Finally, concluding remarks are reported.

2. Methodology

2.1. Machine learning characterisation

Machine learning consists of using data that describe the features and solution(s) of a problem to characterise the problem itself, facilitating the development of prediction abilities. The amount, quality and representativeness of the explanatory variables (or data features) available to train the model are critical aspects for ensuring the performance of such characterisation. XGBoost (standing for extreme gradient boosting) is a relatively recent and powerful evolution of ensemble learning algorithms proposed by Chen and Guestrin (2016), which consists of an iterative boosting process using the gradient descent architecture. In other words, while more established ensemble learning algorithms such as random forests (Breiman, 2001) resort to a so-called bagging method, which aggregates the predictions of weak learners (models with poor accuracy) to obtain one model with better performance, XGBoost resorts to a boosting method which adds a new weak learner (binary tree or logistic regression) at each iteration of the

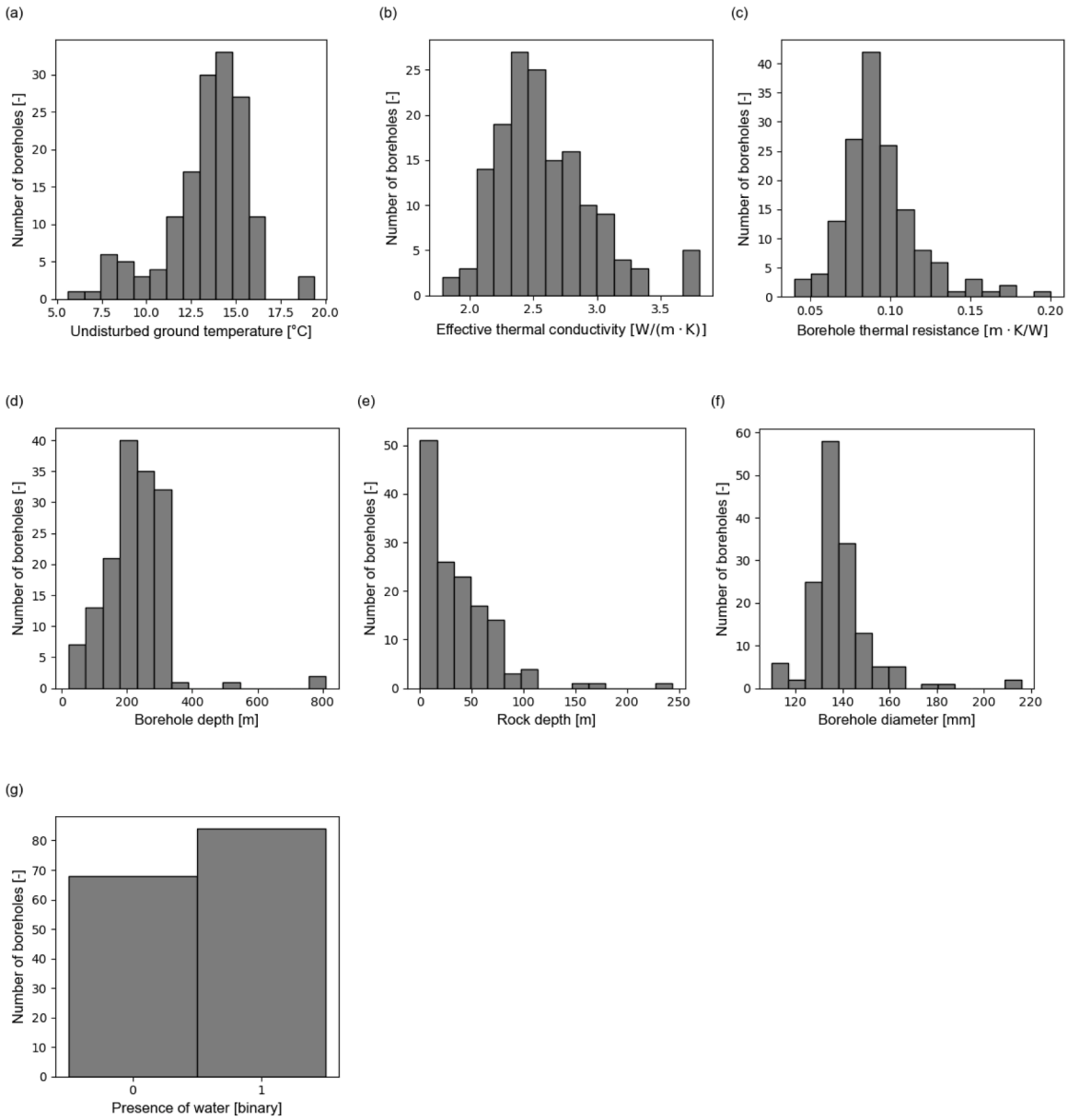

Fig. 2. Distribution of information extracted from TRT reports: (a) undisturbed ground temperature, (b) ground effective thermal conductivity, (c) borehole thermal resistance, (d) borehole depth, (e) rock depth, (f) borehole diameter, and (g) presence of water during drilling.

training process. This approach aims at minimising the residuals of the last iteration. The main advantages associated with using the XGBoost consists in its rapid training speed compared to random forest and its regularisation that helps reducing variance. However, using the XGBoost also has some disadvantages, mainly related to its complexity and difficulty to be tuned. With these premises, the performance of XGBoost is generally more satisfactory than random forest.

In the present study, the XGBoost model is implemented based on the Scikit-Learn Python library for machine learning. Each data set is split into training data (80% of the overall dataset) and test data (the remaining 20% of the overall dataset). The representativeness of the test data respective to the training data is validated by comparing the variances of the two datasets for the three target variables. For both models the hyperparameters are optimised and the training is performed according to the methodology presented in Section 3.1. The quality of the prediction is evaluated with the testing error on the test data, i.e., between the predicted values and the actual observed values. The mean absolute error, *MAE*, and root-mean-square error, *RMSE*, are both widely used error metrics measuring distances in regression problems. They both express a measure of errors between pairs of values representing the same phenomenon. In this case, they express a comparison between the predicted values and the actual observed values. The *MAE* is computed as the average of the absolute error between the predicted values and the actual observed values over the whole test set. The *RMSE* is computed as the square root of the average of squared errors. *MAE* and *RMSE* are thus calculated as follows, respectively:

$$MAE = \frac{1}{n}\sum_{i=1}^{n}\left|y_i - \widehat{y}_i\right| \tag{1}$$

$$RMSE = \sqrt{\sum_{i=1}^{n}\frac{\left(\widehat{y}_i - y_i\right)^2}{n}} \tag{2}$$

with $\widehat{y}_i$ representing the actual value, y_i representing the prediction and n representing the test dataset size. It is important to note that while

these errors are both insightful indicators of the quality of the prediction, by expressing average prediction errors in a manner indifferent to the direction of the error, the *RMSE* penalises large errors and thus increases as the variance associated with the frequency distribution of the error magnitudes increases. This latter aspect is essential in this case, as the objective of the model is to provide design parameters. Thus, significant errors should preferably be avoided.

2.1.1. Dataset

The complete dataset at each point of the study was divided between explanatory variables (or features) and targets. The TRT spatial distribution is presented in Fig. 1. The TRTs are unevenly distributed and correspond to the most populated areas of central and western Switzerland, such as the Geneva Lake region and the cities of Fribourg and Bern.

2.1.1.1. Explanatory variables. The selection of the explanatory variables (or features) is paramount when developing a machine learning model. In this case, the challenge of selecting common explanatory variables for the multitude of the TRT reports made available by companies and cantons (administrative authorities) of central and western Switzerland arose. For example, while some TRT reports included information about the presence and significance of groundwater flow, this was not a common feature. Therefore, this explanatory variable could not be considered as a generalized feature of the developed model.

The struggle of determining a consistent and meaningful dataset for the investigated TRT reports, which is a common feature of all problems dealing with data science in practical engineering applications and certainly of subsurface-related characterisations, was overcome by finding two sets of common explanatory variables to the TRT reports for the 174 available boreholes. A first set of features was related to the borehole location (e.g., the geographical coordinates and depth of the test borehole). A second set of features was related to characteristics of the available boreholes (e.g., borehole diameter, depth of bedrock). It is worth noting that this second set of explanatory variables explicitly included little information about hydrogeological conditions and the presence of groundwater flow, which are renowned to play a significant role in the determination of design parameters targeted by TRTs (Laloui and Rotta Loria, 2019), such as undisturbed ground temperature and ground effective thermal conductivity. Nevertheless, it was considered that the results provided in TRT reports for different borehole locations would have inherently and implicitly included information about hydrogeology and groundwater. As a result, it was hypothesized that the employed machine learning approach would have been capable to account for such important aspects of the problem when developing site-specific and regional-scale prediction upon appropriate training, associating this parameter to another relevant explanatory variable, such as the borehole location.

In an effort to enrich the available dataset with information that could have best served the prediction of the targeted design parameters for BHE applications, some information about the major ground characteristics and geological conditions was included in the dataset. In fact, information on the surface geological formations and materials at the national level was derived from the GK500 (or GeoCover500) dataset provided by the Swiss Federal Office for Topography (Swisstopo) and used by Assouline et al. (2019) for similar applications. The data were available in a GIS vector polygon format, with each polygon representing the boundaries of a surface geological formation and including various pieces of information about the formation. The features extracted from the GK500 dataset were all categorical (class-based) features, which were converted into real values using a "one hot encoding" approach consisting of the creation of as many binary features as there are classes and labelling each feature with 0 or 1 (1 if the point belongs to the class for this variable, 0 if it does not). It should be noted that the geological information extracted from the GK500, once projected on each borehole, did not introduce much variability between neighbouring boreholes compared to the large variety of classes available in the GK500, because the available boreholes are often geographically close. However, inclusion of such information in the dataset was considered relevant for two reasons: first, to highlight the relative significance in the accuracy of the developed predictions as compared to the explanatory variables pertaining to the two aforementioned sets of features (e.g., geographical coordinates of the boreholes); second, to enhance in any case the developed machine learning predictions.

Table 1
Data type and content.

Type	Content
Borehole location	Borehole coordinate X [m], Borehole coordinate Y [m], Borehole altitude Z [m], Borehole depth [m]
Borehole characteristics	Presence of water inflow during drilling [yes/no], Bedrock depth [m], Borehole diameter [mm]*
Surface geological information (GK500)	Geological formation: quaternary, tertiary, etc., Rock type: sedimentary, igneous, and metamorphic., Lithology class: sand, silt, clay, limestone, gneiss, gabbro, basalt, andesite, etc., Hydrological characteristics: surface water, presence of aquifers, etc., Productivity of aquifers: saturation state from 2 to 10 m, from 10 to 20 m, etc.

*This variable is used only for borehole thermal resistance predictions.

Table 2
Experimental variance of the train and test datasets.

Dataset	Variance		
	Undisturbed ground temperature	Ground effective thermal conductivity	Borehole thermal resistance
Train (80%)	5.26	0.14	0.00054
Test (20%)	5.33	0.13	0.00059

2.1.1.2. Target variables. The target variables are the design parameters obtained from a TRT and comprise (i) the undisturbed ground temperature, (ii) the ground effective thermal conductivity and (iii) the borehole thermal resistance. Fig. 2 shows the distribution of the TRT results encountered in the dataset. When the bedrock was not reached during drilling (11 boreholes concerned), the value 999 m was considered in the model (this value is not represented in Fig. 2(d)).

As previously stated, the available dataset was split into training data (80% of the overall dataset) and test data (the remaining 20% of the overall dataset). The representativeness of the test data with respect to the train data should be validated by comparing the variances of the two datasets for the three target variables. Those variances are presented in Table 2 and validate the representativeness of the test data respectively to the train data.

The training of the model serves a twofold objective. A first model is trained with the aim to provide a site-specific substitute for a TRT, thus benefiting from all the data available presented in Table 1, which comprise the surface geological information, the borehole location, and the borehole characteristics (after the drilling of the first in situ borehole has been completed). It should be noted that to avoid being confronted to incomplete data, only the information provided in every test report was considered to build the dataset A second model is trained to map thermo-physical characteristics at the regional scale, thus not benefiting

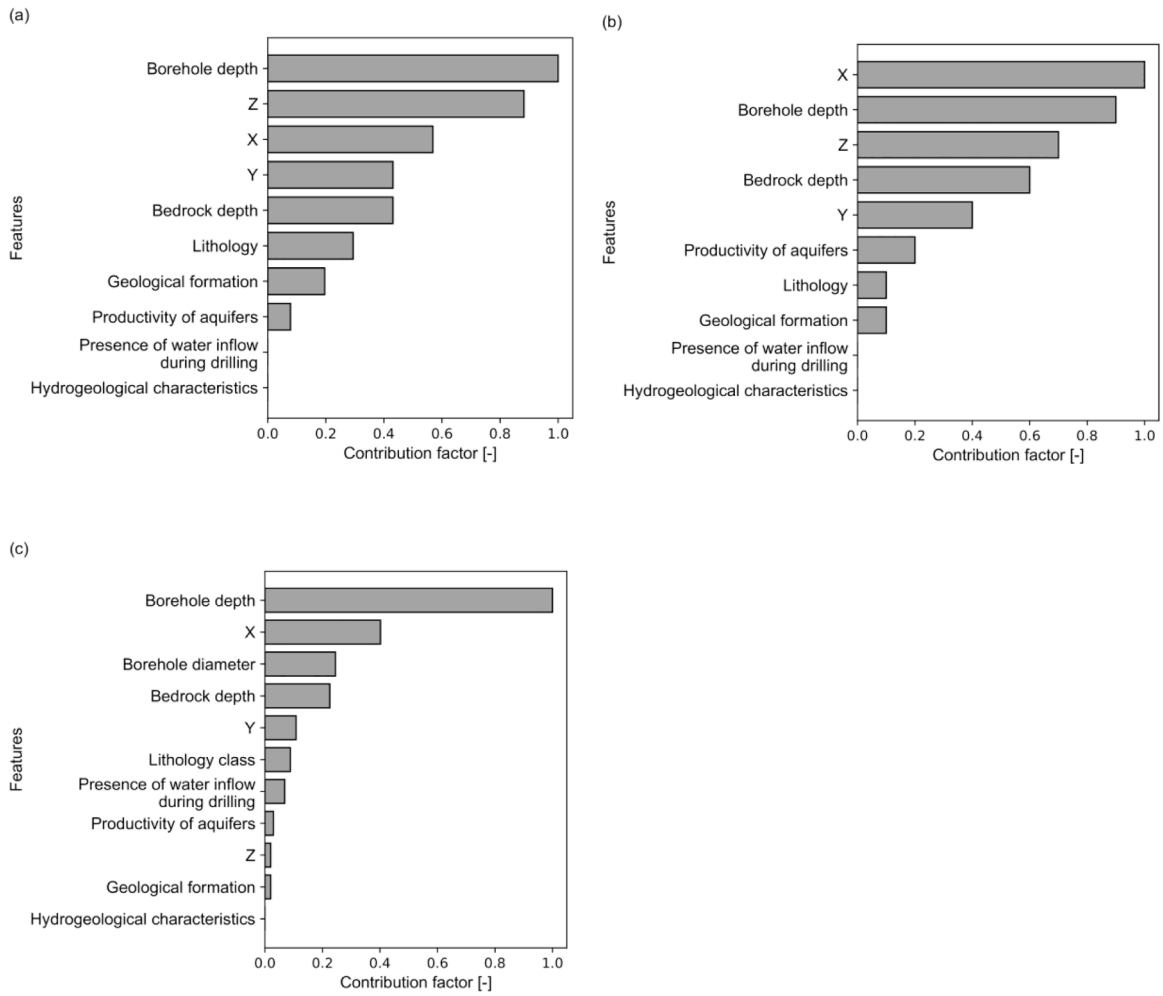

Fig. 3. Feature contribution factors for the site-specific prediction of (a) the undisturbed ground temperature, (b) the ground effective thermal conductivity, and (c) the borehole thermal resistance.

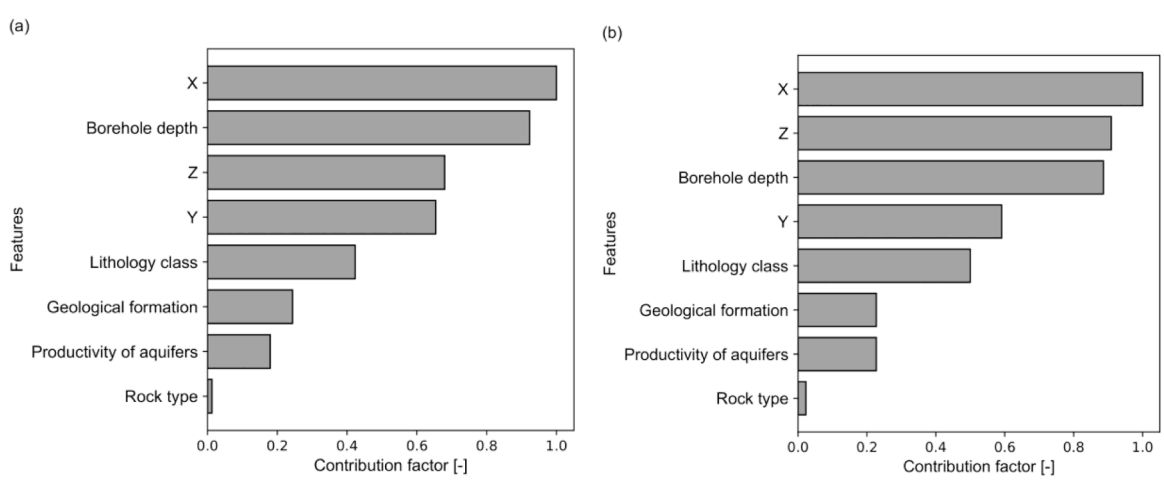

Fig. 4. Feature contribution factors for the regional-scale prediction of (a) the undisturbed ground temperature and (b) the ground effective thermal conductivity.

Table 3
Model quality for the site-specific prediction of TRT results.

Predicted variable	*MAE*	*RMSE*
Undisturbed ground temperature [°C]	0.655	0.895
Ground effective thermal conductivity [W /(m·K)]	0.194	0.263
Borehole thermal resistance [m·K /W]	0.0164	0.0218

from the in situ borehole characteristics but only from the surface geological information and the borehole location presented in Table 1. As the borehole thermal resistance is greatly influenced by the borehole geometry (length, diameter, and pipe configuration of the heat exchanger), mapping this characteristic at a regional scale is considered inappropriate and irrelevant in this context. To account for vertical variability, the effective thermal conductivity is estimated at different depths (100 m and 200 m).

3. Results

3.1. Model training

A single method is used twice to train both models (for site-specific and regional scale predictions), which only differ in terms of the employed training dataset. The construction of each model consists in the optimisation of hyperparameters and the training of the model, which are realised simultaneously, with the objective to minimise the prediction error (*RMSE*, calculated as in Eq. (2)). In the case of XGBoost, the model hyperparameters, i.e., the properties that govern the entire training process, comprise:

- colsample_bytree: subsampling ratio of columns for every tree constructed,
- learning_rate: shrinking ratio of the feature weights at each boosting steps, it helps keeping the process more conservative,
- n_estimators: number of decision trees used,
- max_depth: maximum depth of a tree,
- subsample: subsampling ratio of the training. The dataset is subsampled every iteration of the boosting process to prevent overfitting,
- gamma: minimum loss reduction required to make a new partition on a leaf node of a tree.

500 models with different sets of hyperparameters are trained using 5-split cross-validation on the training set (80% of the whole dataset). The 5-split cross-validation consists of training and evaluating each model (or set of hyperparameters) on different train/test distributions

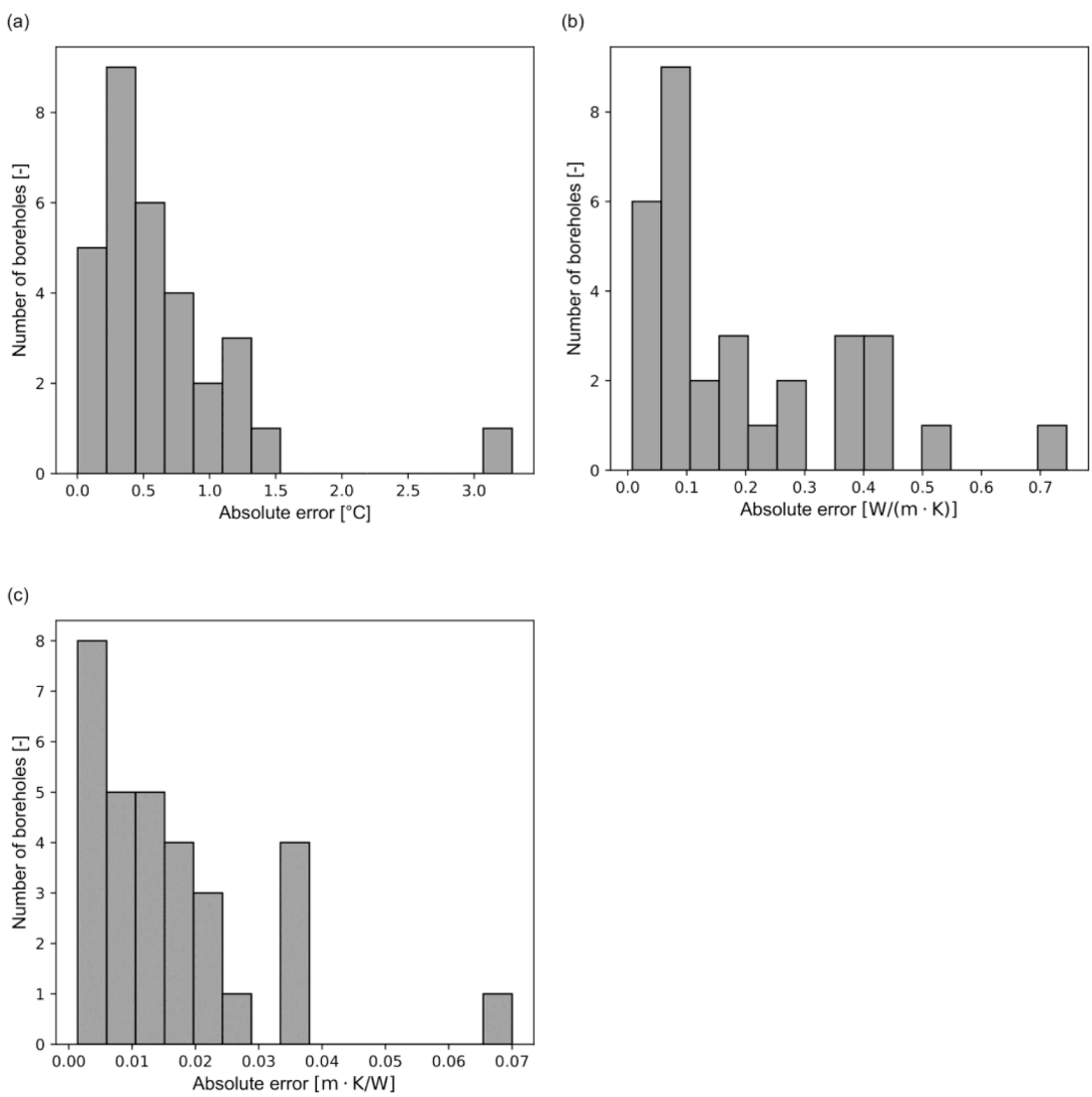

Fig. 5. Distribution of absolute errors for the site-specific prediction of (a) the undisturbed ground temperature, (b) the ground effective thermal conductivity, and (c) the borehole thermal resistance.

Table 4
Quality of predictions for the regional-scale prediction of the thermo-physical mapping of the shallow underground.

Predicted variable	*MAE*	*RMSE*
Undisturbed ground temperature [°C]	0.776	1.238
Ground effective thermal conductivity [W/(m·K)]	0.258	0.370

and retain the best average model on these splits to mitigate the risk of overfitting. Five splits were used to keep the 80-20% repartition of the training-test dataset. The best performing set of hyperparameters is derived from this optimisation process.

The contribution factors represent the relative usage of each feature in the regressors built in the XGBoost model. The higher is the contribution factor, the more relevant the feature for the regression will be, and hence, the higher the dependency of the prediction on this feature. As XGBoost is based on decision trees regressors, the contribution factor is obtained by counting how many times each feature is used as a decision criterion on nodes composing the multitude of trees that were trained to build the model. This can be easily obtained using the plot_importance() method of the XGBoost library. The contribution factors obtained for the site-specific prediction are presented in Fig. 3 (model trained with all the available data reported in Table 1). The contribution factors obtained for the regional-scale prediction are presented in Fig. 4 (model trained without in situ borehole characteristics) with a normalised value ranging from 0 to 1 for the sake of comparison. A contribution factor of 0 means that the feature was never selected by the model.

Local considerations (embedded in the borehole location) play a major role in the prediction of the undisturbed ground temperature and the ground effective thermal conductivity, corroborating that in the absence of in situ hydrogeological measurement, the employed machine learning approach derives information about the local hydrogeological conditions from such data rather than from the actual yet very sparse hydrogeological information supplied to the algorithm through the GK500 dataset. The borehole geometry, including its depth and diameter, logically play a significant role for the thermal resistance estimation in the case of a site-specific prediction only.

Although the contributing factors are understandably a direct consequence of the influence of a given feature on the predicted variable, their magnitude should be carefully considered and should account for the manner the variable is included in the dataset. Typically, one could infer that a null contribution factor means that the feature does not have any influence on the predicted variable. However, this means that the way the type of information provided to the model does not allow to consider the influence of the specific considered feature properly. In other words, the fact that contribution factors close to zero are observed in this study for the hydrogeological characteristics does not imply that hydrogeology is not an important feature in the estimation of the undisturbed ground temperature or the ground effective thermal conductivity. Instead, as mentioned above, this result simply highlights that the level of detail and information embedded in the data supplied to the algorithm for the variable "hydrogeological characteristics" is scarce for the predictions made (e.g., as compared to their resolution). As a result, the information that the algorithm derives in an implicit manner from the borehole coordinates appears to result more effective for the (implicit) consideration of the local hydrogeological subsurface conditions.

3.1.1. *Site-specific predictions*

This section presents the prediction obtained with model trained with all the available data presented in Table 1, comprising the surface geological information, the borehole conditions and the borehole characteristics (after the drilling of the first in situ borehole is concluded), to provide a site-specific substitute for a TRT. The quality of the site-specific predictions for the (i) undisturbed ground temperature, (ii) ground effective thermal conductivity and (iii) borehole thermal resistance compared with actual testing values is shown in Table 3.

The magnitude of the errors observed in Table 3 is very satisfactory for BHE applications. As an example, the Swiss Norm for geothermal probes (SIA, 2010) considers a similar range of variability (up to 1 W/(m·K)) for the thermal conductivity of soils and rocks. Moreover, as the exact knowledge of some testing parameters suffers from uncertainties (e.g., the exact injected power over time), TRT results are typically provided with an error to consider in the calculation, on average, 0.21 °C for the undisturbed ground temperature, 0.19 W/(m·K) for the ground effective thermal conductivity and 0.01 m·K/W for the

Table 5
Variance in prediction errors for site-specific predictions and regional-scale predictions of thermo-physical characteristics.

Predicted variable	Variance in errors	
	Site-specific prediction	Regional-scale prediction
Undisturbed ground temperature	0.37	0.88
Ground effective thermal conductivity	0.03	0.08

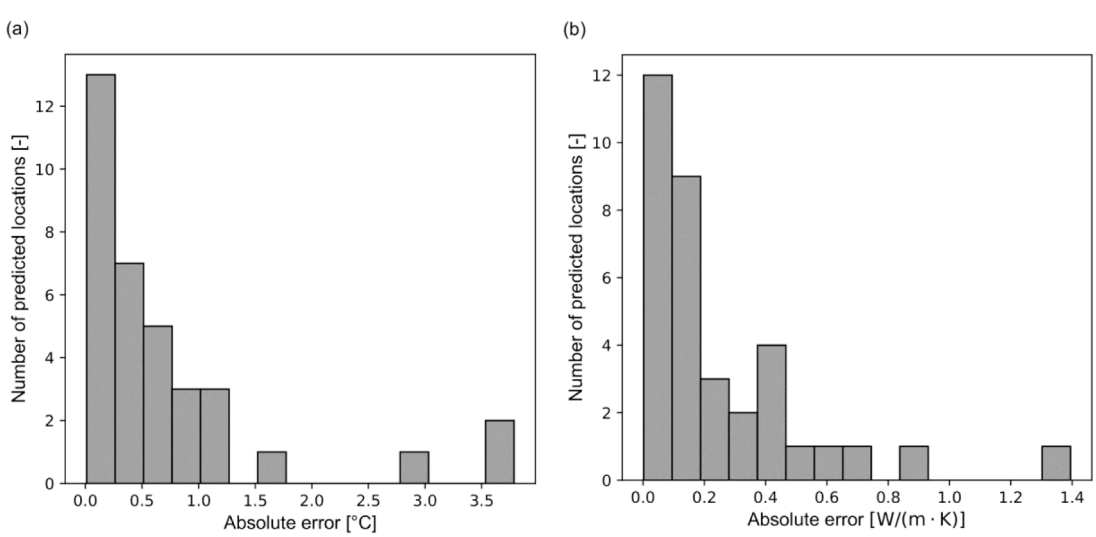

Fig. 6. Distribution of absolute errors for the regional-scale prediction of (a) the undisturbed ground temperature and (b) the ground effective thermal conductivity.

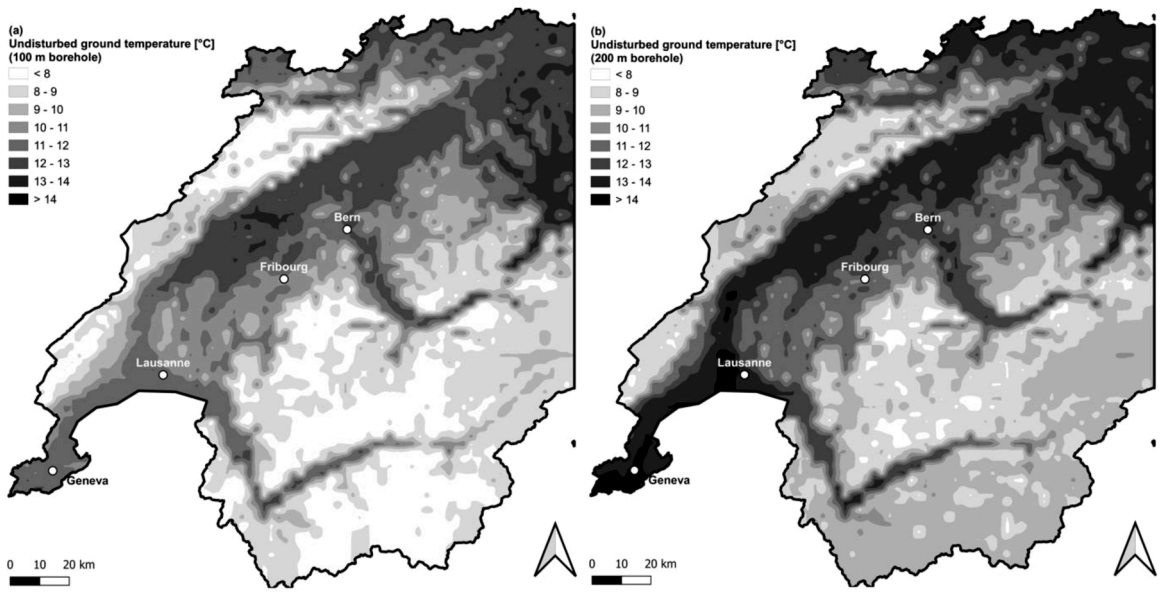

Fig. 7. Predicted average undisturbed ground temperature at (a) 100 m and (b) 200 m.

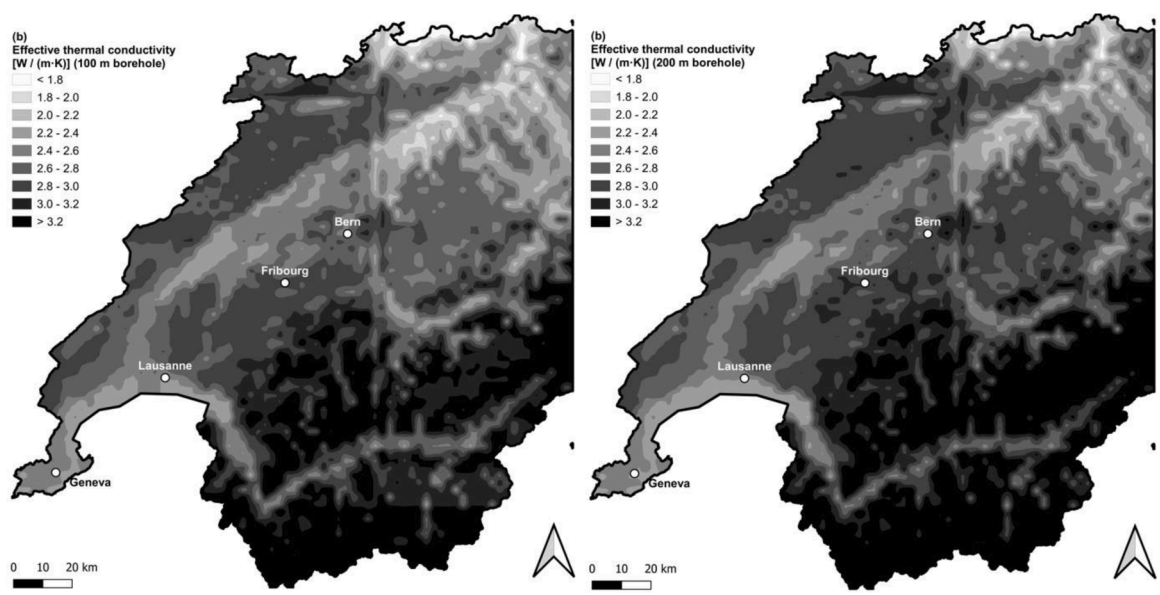

Fig. 8. Predicted ground effective thermal conductivity at (a) 100 m and (b) 200 m.

borehole thermal resistance (among the TRTs gathered in the framework of this study). The similarity between the accuracies of actual in situ testing and prediction emphasizes the performance of the model. Also, the similarities observed between the *MAE* and *RMSE* for the prediction of the undisturbed ground temperature, ground effective thermal conductivity and borehole thermal resistance indicate that the variance in error is low, as illustrated in Fig. 5 and presented in Table 5.

3.1.2. Regional-scale predictions

This section presents the prediction obtained with the model trained without benefiting from the in situ borehole characteristics (which may be recovered only after an actual in situ borehole has been completed) but only from the surface geological information and the borehole conditions presented in Table 1 to map the thermo-physical characteristics at a regional scale. The quality of the predictions of the undisturbed ground temperature and ground effective thermal conductivity compared to actual testing values is shown in Table 4.

As the model does not benefit from in situ borehole characteristics, the regional-scale predictions are of a lesser quality than the site-specific predictions presented in the previous section. Nevertheless, the model still provides very satisfactory predictions according to the considerations on the tolerable range of uncertainty presented in the previous section. Similarly, the *MAE* and *RMSE* indicate that the variance in error is low for the prediction of the ground effective thermal conductivity, while it is higher for the undisturbed ground temperature. These aspects are also highlighted in Fig. 6. Overall, the variance in error is more significant in the case of a regional-scale prediction than a site-specific prediction benefitting from in situ borehole characteristics, as shown in Table 5.

Once the capability of the model to grasp the considered problem was assessed, 20% of the dataset previously kept for testing was integrated to the training dataset to produce the regional-scale predictions of the undisturbed ground temperature and the ground effective thermal conductivity reported in Figs. 7 and 8, respectively. In this regard, the errors presented in Table 4 using splits between training and test set should be considered as upper boundaries. Predictions are reported for

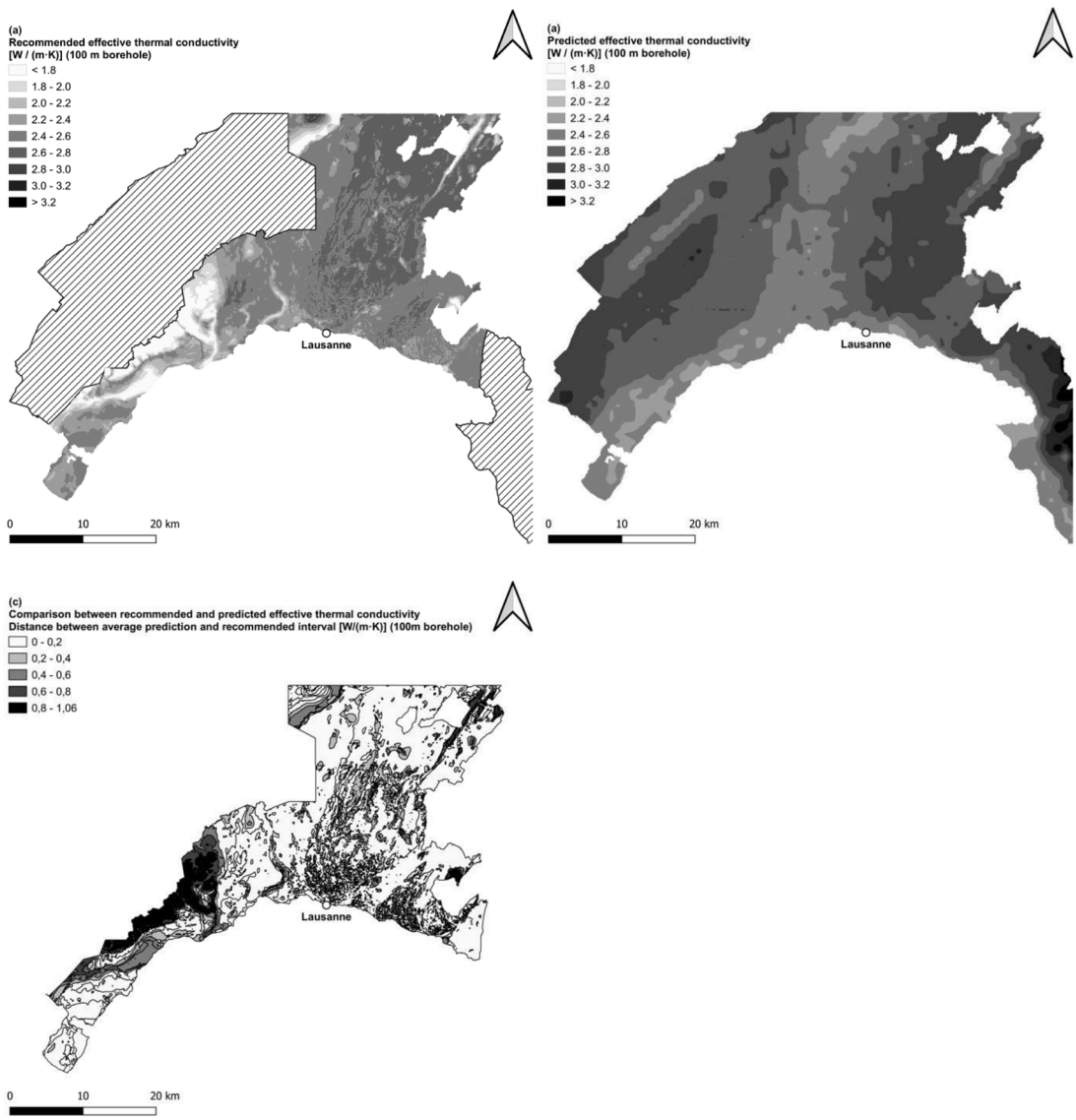

Fig. 9. Evaluation of the ground effective thermal conductivity for a 100-metre borehole in the state of Vaud according to (a) the state administration and (b) the model and (c) absolute errors between values from both sources.

100- and 200-metre boreholes as they represent common depths of application for such technologies in Switzerland and abroad.

A way to assess the quality of the ground effective thermal conductivity mapped by the model is to compare the similarities with conductivity maps provided by state administrations. These maps, presented and compared to the model for 100 metre and 200 metre boreholes in Figs. 9 and 10, respectively, are built combining the national geological information at different depths with the values of ground effective thermal conductivity for several types of soil and rocks provided by the Swiss Norm (SIA, 2010). The dashed areas represent the zones where BHEs are excluded due to regulations on underground water resources.

The comparison presented in Figs. 9 and 10 highlights the similarities between the traditional methods and the model, and validates the use of a machine learning method to interpret national geological information combined with in situ testing results for predicting thermo-physical characteristics at different depths on a regional scale. It is worth noting that the model evaluates the ground effective thermal conductivity with a greater precision for larger depths, and that logically, the model performs better for areas benefiting from more training data, corresponding to the most populated areas according to Fig. 1.

4. Discussion

This work aims to take advantage of the experience gained through the past testing of the shallow underground of a given area to characterise future sites of any region or country, without resorting to additional in situ testing. Based on the results obtained in this study, machine learning appears to offer a powerful means to account for past experience in a practical way, using the data describing the features and solution(s) of any considered problem to characterise the problem itself and serve accurate predictions. In this sense, the model developed in this study may be considered like a geologist with substantial knowledge, with the ability to quantify the thermo-physical characteristics of the shallow subsurface for local sites and regional areas.

The challenges encountered in this study for identifying a common and meaningful dataset for the problem addressed indeed represents an

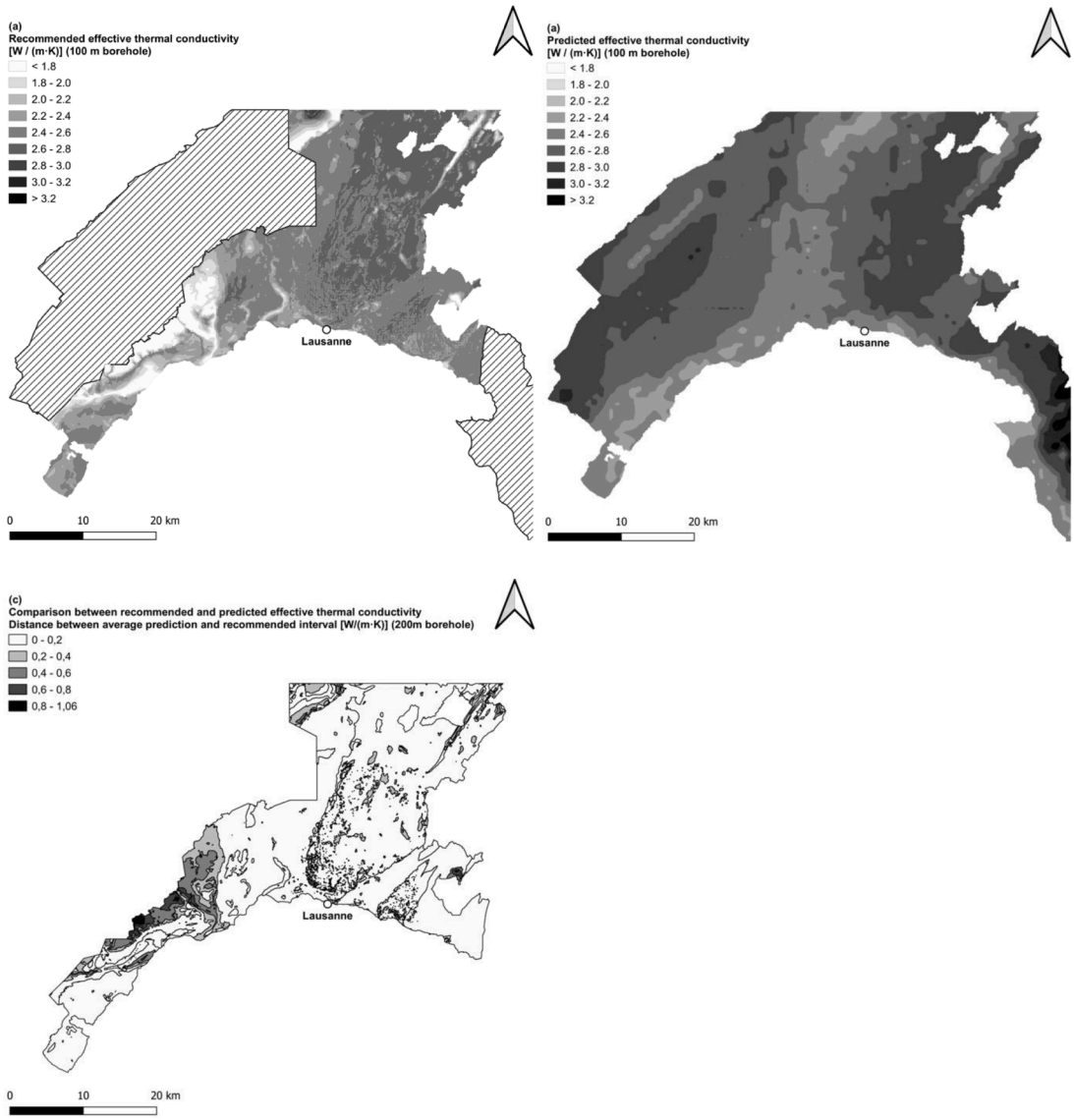

Fig. 10. Evaluation of the ground effective thermal conductivity for a 200-metre borehole in the state of Vaud according to (a) the state administration and (b) the model and (c) absolute errors between values from both sources.

intrinsic issue of all works related to data science in practical engineering applications. The approach used in this study to select the explanatory variables was based on the experience of the authors in this field, but also forced by the availability of given data (e.g., specific coordinates of the boreholes instead of specific hydrogeological characteristics). Other approaches could indeed be considered to select dataset for predictions such as those targeted by this work. For example, considering detailed data about the specific hydrogeological features of the investigated area (groundwater flow rate, depths at which groundwater flow was encountered, etc.) would appear advantageous for trainings and predictions of undisturbed ground temperature and ground effective thermal conductivity, rather than the coordinates of the boreholes from which these data are determined through TRTs. Such an approach may lead to predictions characterised by a greater accuracy than those reported here and deserves further investigations in the future.

5. Concluding remarks

For the first time, this paper investigated a machine learning approach for providing accurate and effective predictions of critical thermo-physical characteristics of the underground for the analysis and design of shallow geothermal heat exchangers: (i) the undisturbed ground temperature, (ii) the ground effective thermal conductivity and (iii) the borehole thermal resistance. The results presented in this work underline a highly satisfactory capability of the considered machine learning approach to estimate the aforementioned thermo-physical characteristics of the subsurface, from local sites to regional areas. Comparisons with actual testing results of undisturbed ground temperature, ground effective thermal conductivity, and borehole thermal resistance highlight prediction errors of less than 0.7 °C, 0.2 W/(m·K) and 0.02 m·K/W, respectively.

In the future, the model investigated in this work could represent a major opportunity for a partial or complete substitute for thermal response tests, which have been historically run to determine the in situ thermo-physical characteristics of the underground for most of the analyses and engineering designs of shallow geothermal systems. The analysed machine learning approach could specifically serve administrative authorities to map design parameters, characteristics, and heat exchange potential for geothermal or other geoenergy applications, from local to very large spatial scales. The satisfactory results obtained in this paper, along with the relatively limited number of explanatory variables used, provide significant confidence in the above vision. Such

a vision encourages the digitalization and pooling of available thermal response testing results, so that highly accurate predictions of the subsurface thermo-physical characteristics could be obtained in the future through computational predictions that will resort to decreasing or no additional thermal response test results.

CRediT authorship contribution statement

Paul Bourhis: Formal analysis, Software, Methodology. **Benoît Cousin:** Conceptualization, Methodology, Investigation, Funding acquisition. **Alessandro F. Rotta Loria:** Validation, Visualization. **Lyesse Laloui:** Supervision, Project administration.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgement

This work was supported by the Swiss National Science Foundation (grant number 40B1-0_189766) and was possible thanks to the TRT data made available by the State of Vaud (DGE/GEODE), Geoazimut and Geotest.

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