Deep learning and geochemical modelling as tools for solute geothermometry

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Keywords: solute geothermometry, multicomponent geothermometer, artificial neural network geothermometer

ABSTRACT

Geothermometry is constituted one of the most important geochemical tools for reservoir exploration and development. Solute geothermometers are used to estimate the temperature in the subsurface. Therefore, the chemical composition of a discharging geothermal fluid is used to infer the temperature of the reservoir. Changes in the chemical composition because of boiling, degassing, and dilution are disturbing the equilibrium state within the fluid leading to uncertainties in the temperature estimation. Especially, the pH value, the aluminium concentration, as well as boiling and dilution are parameters prone to changes. These parameters are elaborated in the geochemical modelling process to optimise these values to fit their in-situ reservoir conditions again. This geochemical modelling method can be used for multicomponent geothermometers leading to more robust and precise temperature estimations. However, this process is time-consuming, and geochemical as well as mineralogical knowledge is beneficial. Consequently, the field of artificial intelligence offers powerful methods to solve complex issues, even considering multiple unknowns. Therefore, a new solute geothermometer based on a deep learning algorithm is developed. This neural solute geothermometer is tested and compared to the optimised multicomponent geothermometer and in-situ temperature measurements concluding in a new generation of solute geothermometer as precise as an optimised multicomponent geothermometer but much easier and faster in its applicability.

1. INTRODUCTION

The temperature determination of the reservoir is a major factor in the assessment of geothermal reservoirs, especially during the exploration phase. Solute geothermometry can provide such temperature estimations assuming temperature-dependent equilibrium reactions between the geothermal fluid and the host rock minerals. Originally, conventional geothermometers were introduced using cation ratios or single mineral phases for temperature estimation (Fournier and Truesdell 1973, Giggenbach 1988, Arnórsson 2000). Followed by a more robust method introduced by Reed and Spycher (1984) using temperature-dependent saturation indices of multiple mineral phases for reservoir temperature estimation. This led to the development of multicomponent geothermometers such as MulT_predict, GeoT, and RTEst (Ystroem et al. 2020, Palmer 2014, Spycher et al. 2014). In an ongoing development, optimisation processes are implemented to improve the accuracy of these multicomponent geothermometers (Spycher et al. 2016, Ystroem et al. 2021). Especially, steam loss and dilution, as well as trace element concentrations (e.g. Al, Fe, or Mg), and pH value (e.g. degassing) are prone to perturbation of the *in-situ* equilibrium state, which therefore is back-calculated within the different multicomponent geothermometers. In some cases, these optimisation processes are computationally intensive, when applied interdependently while there are unknowns like the mineralogy of the reservoir (Ystroem et al. 2022). Thus, a new solute neural geothermometer is developed. Artificial neural networks (ANN) are designed to solve complex issues incorporating unknowns (Goodfellow et al. 2016). In addition, a trained network is able to handle a large amount of data efficiently conducting reservoir temperatures estimations. Further, both methodologies are compared to evaluate the temperature estimations. Therefore, a case study of temperature estimations is conducted based on high-quality data from Iceland. The dataset consists of fluid samples from geothermal wells and their in-situ temperature measurements are given by Arnórsson et al. (1983), Guðmundsson and Arnórsson (2002), and Óskarsson et al. (2015).

2. METHOD & DATA

Solute geothermometry is based on the temperature-dependent solubility of mineral phases with the surrounding fluid. Under unperturbed conditions, an equilibrium state between the dissolved element concentration of the fluid and the reservoir rock is reached (Fournier and Truesdell 1974). Therefore, element ratios, as well as individual solute mineral phases can be used to determine the temperature of the reservoir.

2.1 Multicomponent geothermometry

To increase the robustness and the precision of geothermometry the solubility of multiple mineral phases can be evaluated simultaneously. In this approach, the saturation indices *SI* of the mineral phases are evaluated over a predefined temperature range (Reed and Spycher 1984). The geochemical equilibrium is reached when the measured ion activity product *IAP* is equal to the temperature-dependent thermodynamic constant *K(T)* [1]. In this case, the *SI* of the mineral phase equals zero (*SI* = 0).

$$SI(T) = \log \frac{IAP}{K(T)} \qquad [1]$$

SI saturation index; *T* temperature; *IAP* ion activity product; *K* thermodynamic equilibrium constant

Immature fluids or secondary processes shift the fluid from its equilibrium state. Especially, secondary processes like phase segregation, boiling, mixing, dilution, as well as precipitation of mineral phases and complex building lead to perturbation and thus to uncertainties in the reservoir temperature prediction (Arnórsson et al. 1990, Cooper et al. 2013, Peiffer et al. 2014, Nitschke et al. 2017). Optimisation processes are able to reconstruct equilibrium state conditions assuming the individual mineral equilibrium temperatures converge to an equal overall reservoir temperature. This is achieved by varying sensitive parameters (pH value, aluminium concentration, and the fluid fraction) interdependently around the initial conditions until a global minimum between the equilibrium states of the mineral phases is reached (Ystroem et al. 2022). Figure 1 illustrates the output of MulT_predict. In a), the saturation indices of the reservoir mineralogy are plotted against temperature. The intersection with the dashed line represents the equilibrium state in the reservoir. Part b) shows the optimisation process; sensitive parameters (pH-value, aluminium concentration, dilution, steam loss) are simultaneously optimised and evaluated. The in-situ reservoir conditions are assumed to be the global minimum of temperature differences between the mineral phases. Plot c) shows the statistical evaluation of the optimisation. The root mean square (RMES), standard deviations (SDEV), median (RMED), and the mean (MEAN) of the saturation indices are calculated and plotted against the temperature. In picture d), the result of the temperature estimation is shown. The box plot comprises the equilibrium temperatures of the best fitting reservoir conditions of the mineral set. Depending on the optimisation range, these optimisation processes can be computational time intensive. For each optimisation step, the calculations are computed interdependently increasing the time by the power of one for each sensitive parameter.

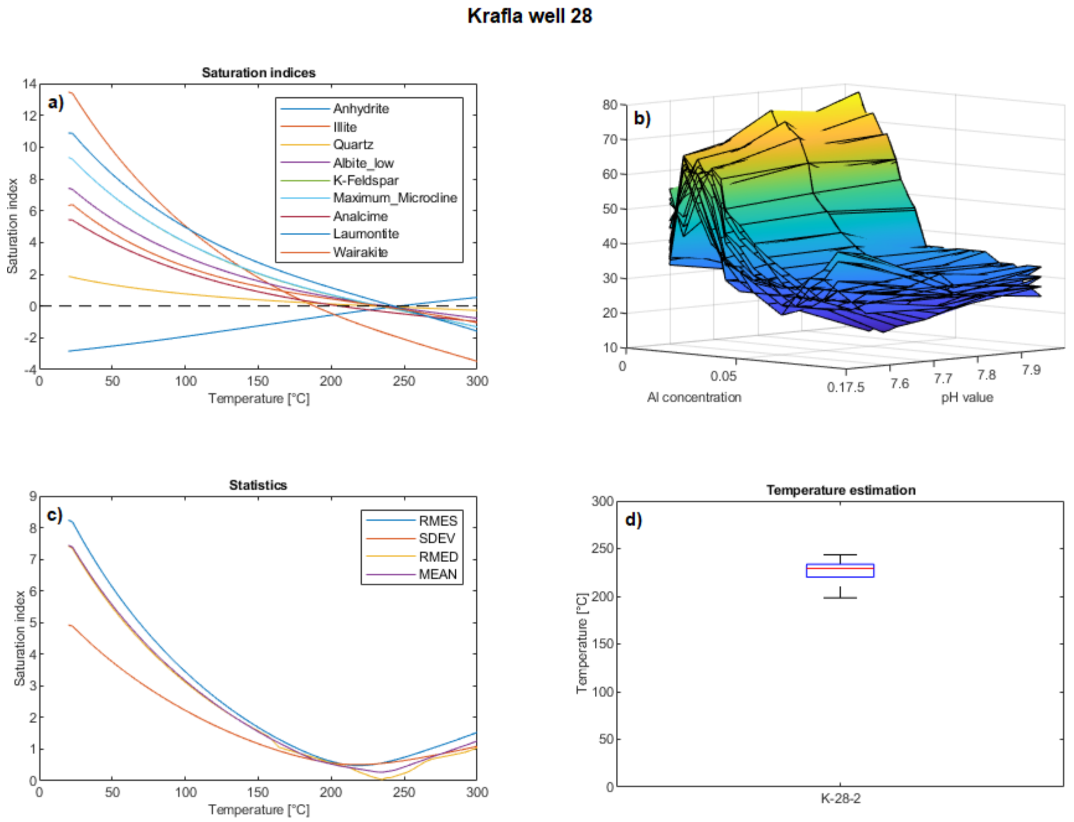

Figure 1: Example of the output of MulT_predict: a) Saturation indices of the reservoir mineralogy against temperature. The intersection with the dashed line represents the equilibrium state in the reservoir. b) Interdependent optimisation process of pH-value, aluminium concentration, dilution, and steam loss, the global minimum represents reservoir conditions of the sensitive parameters. c) Statistical evaluation of the optimisation (root mean square, standard deviations, median, and the mean of the saturation indices). d) Result of the best fitting temperature estimation as a box plot.

2.2 Artificial neural network geothermometry

Regarding the increasing computational time for interdependent optimisation processes of sensitive parameters in multicomponent geothermometry, artificial intelligence can perform calculations even for a large amount of data more efficiently (Goodfellow et al. 2016). Therefore, an artificial neural net (ANN) is trained with geochemical parameters of the fluid composition and in-situ temperature measurements of high-quality fluid data. A dataset of geothermal wells of Iceland given by Arnórsson et al. (1983), Guðmundsson and Arnórsson (2002), and Óskarsson et al. (2015) is compiled as input data for the network. After screening the input data, the selection of geochemical parameters as well as the network structure must be elaborated. Afterward, the network is trained with a majority (70%) of the data. The rest of the data is used for testing (20%) and validation (10%) of the ANN. The goal is to train the ANN to estimate the reservoir temperature without overfitting the algorithm. The result of the training of the ANN, as well as the performance of the trained geothermometer, are illustrated in Figure 2. On the left side of picture a), the mean square error is plotted over the epochs of the training phase. The even trend of the validation curve shows the adaption of the network, while not overfitting the ANN. On the right part of Figure 2 b), the predicted bottom hole temperature is plotted over the measured bottom hole temperature. The blue dots represent the data used for the validation, fitting the trained geothermometer tool with a coefficient of determination R² of 0.978.

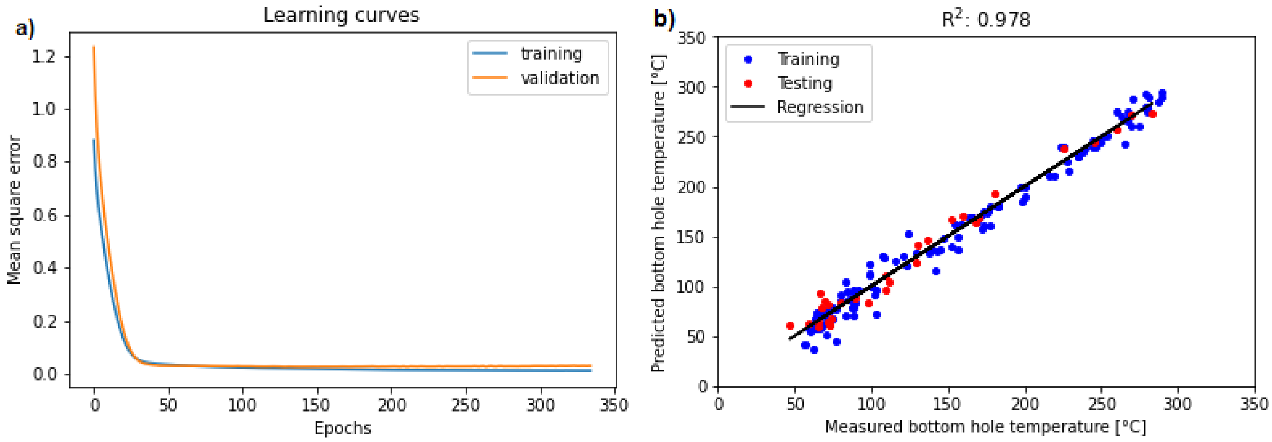

Figure 2: a) Mean square error against the epochs of the training. The early stopping function prevents the ANN from overfitting. b) Predicted versus measured bottom hole temperature. The testing data fits the ANN with a coefficient of determination R² = 0.978.

3. RESULTS

Both methods, the solute multicomponent geothermometer as well as the ANN geothermometer, are used to estimate the temperature of a known reservoir in Iceland. Therefore, four samples of Krafla and Reykjanes are computed. In Figure 3, the resulting temperature estimations are shown. The temperature estimation of the multicomponent geothermometer MulT_predict is visualised by blue box plots while the red line indicates the median temperature. The temperature estimation of the artificial neural network is illustrated by a green circle with an inner black dot. The measured *in-situ* temperatures of the wells are indicated by an orange box given by the inflow temperatures of the geothermal fluid at permeable horizons in the open hole section.

In all cases, the median temperature of the multicomponent geothermometer is fitting the *in-situ* temperatures. For the ANN geothermometer, three of four temperature estimations are matching the measured temperature range. Only for well 28 at Krafla, the ANN is underestimating the temperature by a maximum of 15 Kelvin.

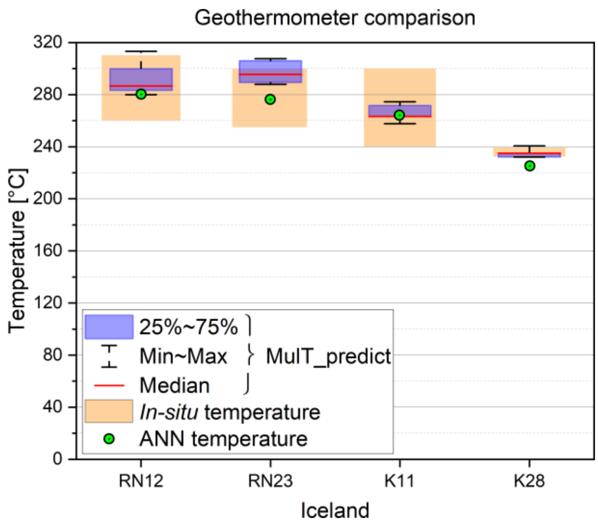

Figure 3: Comparison of multicomponent geothermometer MulT_predict (box plots) and the ANN geothermometer (green circles). The *in-situ* temperature measurement is indicated by the orange box for the four wells in Krafla and Reykjanes, Iceland.

3. DISCUSSION & CONCLUSIONS

Comparing both geothermometer approaches in Figure 3, the solute multicomponent geothermometer is statistically more robust than the artificial neural network. Nevertheless, MulT_predicts' temperature estimations have to be optimised to obtain precise results. Therefore, a mineralogical pre-knowledge of the hosting reservoir rock would be beneficial. In addition, multiple interdependent optimisation processes increase the computational time of the calculations. Regarding this, the newly developed ANN geothermometer can compute temperature estimations more efficiently while handling large amounts of data. In addition, no pre-knowledge nor optimisation is necessary. Nevertheless, the ANN has to be trained with high-quality data containing accurate *in-situ* temperature measurements.

While geochemical modelling of sensitive parameters in solute geothermometry is the key factor for accurate reservoir temperature estimation, a further improved and adequate ANN geothermometer is the next step in the evolution of solute geothermometry.

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Acknowledgments

This study is part of the subtopic "Geoenergy" in the program "MTET - Materials and Technologies for the Energy Transition" of the Helmholtz Association.