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# A digital twin for simulating geochemical processes in geothermal power plants

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## ABSTRACT

In the MALEG project (**Ma**chine **L**earning for **E**nhancing **G**eothermal energy production), artificial intelligence (AI) is used to increase the efficiency of geothermal energy production of power plants. Thus, two digital twins of a geothermal power plant are developed and linked to mimic and operate hydrogeochemical processes throughout the system to decrease thermodynamic losses. First, a digital twin of the geothermal power plant itself is established (cyber-physical system), which includes all sensors and actuators of the power plant. Second, a digital twin of the hydrogeochemical processes (process simulation) within the thermal water cycle is developed.

In terms of the hydrogeochemical process simulation, energy production in geothermal power plants is linked to the inital hydrogeochemical conditions of the fluid. Changes in pressure, temperature, pH, or redox alter the chemical equilibrium of the extracted thermal water, which can lead to processes such as uncontrolled mineral precipitation, degassing, and corrosion. To better map these processes, a digital twin has been developed and applied to several geothermal power plants. The simulations are automatically calculated, transferred, and evaluated. This allows the new hydrogeochemical equilibrium conditions to be directly determined and interpreted as the power plant parameters change. These process simulations, in combination with the cyber-physical system, form the foundation for implementing AI to increase the efficiency of geothermal power plants.

## 1. INTRODUCTION

To improve the efficiency of geothermal energy production, the functional interaction of operating parameters have to be improved (e.g. reduction of pressure maintenance and reinjection temperature). Yet in most cases, the geothermal fluid composition is counteracting this measurments. Whilst pressure relief or cooling, highly mineralised geothermal fluids tend to rise uncontrolled thermodynamic processes (Helgeson et al. 1981). This is a strict limiting factor for the efficient and continuous operation of geothermal power plants. The complex and site-specific hydrochemistry of the fluids complicates the prediction and quantification of fluid perturbation using deterministic geochemical models (Bethke 2008). In the MALEG project, geochemical models are complemented by process simulation, in which hydrogeochemical data is modelled by using a cyber-physical system of the geothermal power plant.

Altering the geochemistry of the fluid due to heat extraction, depressurising, and inhibitor dosing disturbs the equilibrium state within the fluid. In particular, temperature, pressure as well as pH, and redox potential are parameters prone to changes (Reed 1982, Giggenbach 1988). In addition, degassing, mineral extraction, and inhibitor injection change the chemical composition of the thermal fluid. These perturbations of hydrogeochemical equilibrium can lead to problems such as scaling, clogging, and corrosion within the geothermal power plant respectively the reservoir (Brown 2013, Mundhenk et al. 2013, Nitschke et al. 2014).
The aim of the digital twin is the process simulation of the hydrogeochemical environment of the site-specific power plant, which is calculated using PhreeqC as a deterministic model (Parkhurst and Appelo 2013). The variation of geochemical parameters (temperature, pressure, pH, redox) pre-calculates thermodynamic changes of the fluid chemistry (Ystroem et al. 2021). The results of the iterations are used to decrease or mitigate the disadvantages of the usage of geothermal brine and additionally find the potential to increase the efficiency of the power plant. Thereof, a site-specific process simulation database is created, which is used to train an AI to identify the most effective production parameters (Dashti et al. in review).

## 2. METHODS

The digital twin of process simulation is based on a newly developed thermodynamic database (Trumpp et al. in preparation). The database contains revised and updated thermodynamic data of 21 mineral phases for the calculation of solubilities, which have been validated against experimental data. To fit geothermal purposes, the most important secondary mineral phases are used to determine the corrosion, precipitation, and degassing potentials. To calculate possible hydrogeochemical power plant processes (e.g. scaling, corrosion, or degassing potentials), the deterministic model of PhreeqC (Parkhurst and Appelo 2013) is used. These process simulations are based on the site-specific fluid characterisation of three geothermal power plants located in Haag am Hausruck (Austria), Unterschleißheim (Germany), and Gülpinar (Türkiye). Fluid samples were collected at each power plant at multiple locations along the thermal water cycle. Thereof, the operating parameters of the power plant (e.g. temperature, pressure, flow rate) and the chemical composition of the fluid are matched at each location. Those data form the foundation of the site-specific implementation of the hydrogeochemical process simulation. For the tool, MATLAB (MATLAB 2024) is coupled to IPhreeqc (3.7.3 -15968) via a Component Object Model (COM) server, which was introduced by Charlton and Parkhurst (2011).

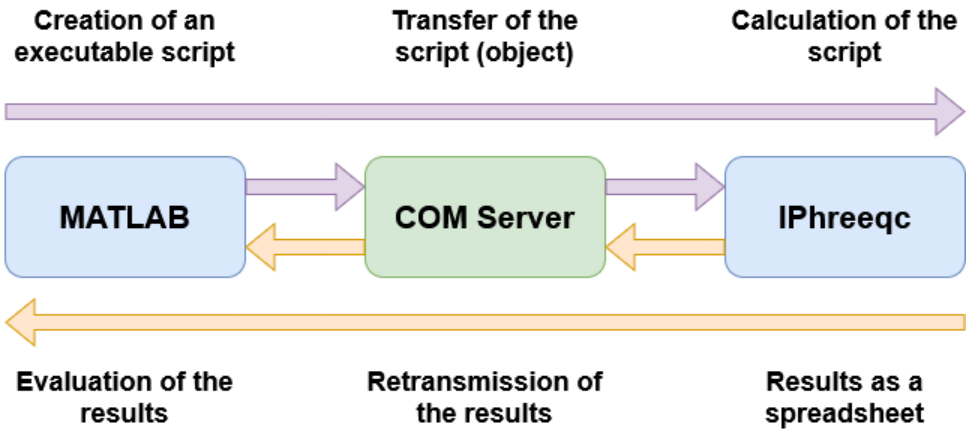


**Figure 1: Flowchart of the process simulation connecting MATLAB and IPhreeqc through a Component Object Model (COM) Server. For each calculation, the initial fluid chemistry is transferred to IPhreeqc to model the thermodynamic processes of the iteration step. The result of the hydrogeochemical modelling is retransmitted to MATLAB for evaluation and merging into a database.**

The MATLAB script communicates via the COM server with IPhreeqc by sending an executable script (Figure 1). Then, the script is conducted and processed in IPhreeqc, calculating the thermodynamic changes of the initial fluid chemistry at operating parameters in the geothermal power plant. Afterward, the results are retransmitted to MATLAB, where the data is merged and saved.

## 3. RESULTS

To simulate thermodynamic processes, the digital twin uses site-specific fluid chemistry as input data to vary possible operating parameters (pressure, temperature, pH, and redox) that occur during power plant operation (Figure 2). These parameter variations can be applied and calculated both individually and in combination with each other. In addition, individual parameters can stay unchanged or can be fixed to specific values to mimic external interference in the chemical system. Both, the operating parameters and the fluid chemistry as well as the solubility products of the secondary mineral phases are calculated and saved for each iteration step (cf. data blocks in Figure 2). Thus, complex, interdependent geochemical processes are simulated and the results are stored in a database. Consequently, the database comprises both chemical data and thermodynamic data linked to each other.

A simple graphical user interface has been implemented to make the program easier to use. A data processing template (hydrogeochemical analysis of the initial fluid chemistry) can be selected and read. In the next step, the user can decide which hydrogeochemical sample is used for the process simulation. Once the selection has been made, the individual operating parameters can be varied or fixed. The number of reaction steps as well as the pressure, temperature, pH, and redox range can be selected. In addition to the number of reaction steps, the interval size can also be adjusted for the individual parameter variations. Once the appropriate selection has been made, the mineral phases are selected from the revised and updated thermodynamic database to be analysed (Trumpp et al. in preparation). By confirming the mineral selection, the script begins to calculate the specified parameter variation step by step. Afterward, these results are compiled. After completion of the script, a database with multidimensional entries is available (Figure 2), which can be used for the implementation and training of an AI (Dashti et al. in review).

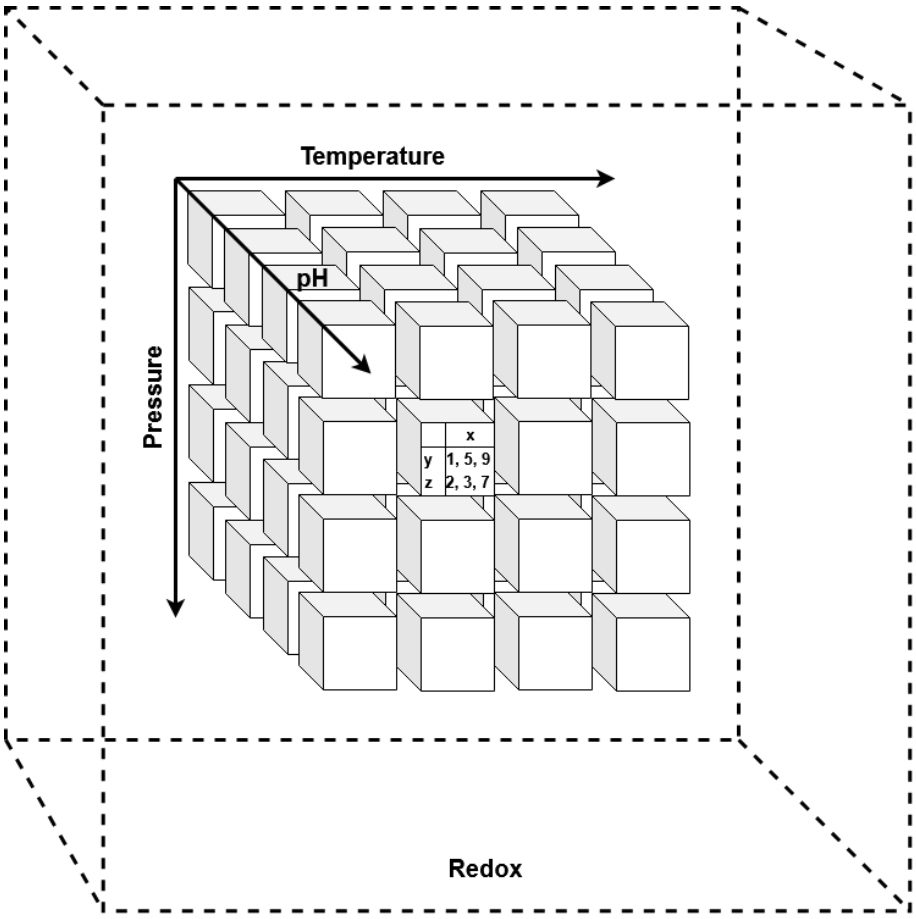


**Figure 2: Schematic illustration of the data output of the process simulation tool. The initial fluid chemistry is altered regarding the operating parameters of the power plant (pressure, temperature, pH, and redox) to mimic interdependent thermodynamic processes within the thermal cycle. Each modelled hydrogeochemical iteration is stored in a table represented as a data block. All data is merged into an elaborate multidimensional database, which is used to train an AI to enhance the efficiency of the power plant and mitigate hydrogeochemical perturbations during production.**

## 4. CONCLUSION

The aim of MALEG is the implementation of an AI to enhance the energy efficiency of geothermal power plants. Thus, an elaborate site-specific database is built. It comprises operating data of the power plant as well as hydrogeochemical data at operating conditions. The database builds the foundation for the training of an AI (Dashti et al. in review). This AI comprises the interdependent thermodynamic processes of the site-specific geothermal fluid chemistry and therefore, can enhance the efficiency of the power plant. In addition, the coupling of the machine learning application with the cyber-physical twin allows the controlling of the hydrogeochemical processes during power plant operation. Thus, the AI independently decreases or mitigates hydrogeochemical perturbations, which lead to uncontrollable processes (scaling, clogging, corrosion) in the thermal water cycle.

## REFERENCES

Bethke, C.M.: Geochemical and Biochemical Reaction Modeling, (2nd Ed.), *Cambridge University Press*, New York, (2008).

Brown, K.: Mineral scaling in geothermal power production, *Geothermal Training Programme Reports 2013*, Nr. **39**, Orkustofnun, Iceland, (2013)

Charlton, S.R., Parkhurst, D.L.: Modules based on the geochemical model PHREEQC for use in scripting and programming languages. *Comput. Geosci*. **37**, (2011), 1653–1663.

Dashti, A., Trumpp, M., Ystroem, L.H., Goldberg, V., Seimetz, N., Nitschke, F.: Interpretable Ensemble Deep Neural Network Training developed for Imbalanced Geochemical Data Distributions. *Natural Resources Research.* In review

Giggenbach, W.F.: Geothermal solute equilibria. Derivation of Na-K-Mg-Ca geoindicators.

*Geochimica et Cosmochimica Acta*, **52**, (1988) 2749–2765.

Helgeson, H.C., Kirkham, D.H., Flowers, G.C.: Theoretical prediction of the thermodynamic behavior of aqueous electrolytes at high pressures and temperatures: IV. Calculation of activity coefficients, osmotic coefficients, and apparent molal and standard and relative partial molal properties to 600°C and 5 kB. *American Journal of Science*, Vol. **281**, (1981), 1249-1516.

MATLAB Version 24.1.0.2537033 (R2024a). *Natick*, Massachusetts: The Mathworks, Inc., (2024).

Mundhenk, N., Huttenloch, P., Kohl, T., Steger, H., Zorn, R.: Metal corrosion in geothermal brine environments of the Upper Rhine graben – Laboratory and on-site studies. *Geothermics*, **46**, (2013), 14-21.

Nitschke, F., Schreiber, J., Kramar, U., Neumann, T.: Formation of alternating layered Ba-Sr-sulfate and Pb-sulfide scaling in the geothermal plant of Soultz-sous-Forêts. *Journal of Mineralogy and Geochemistry*, **191**(2), (2014), 145-156.

Parkhurst, D.L., Appelo, C.A.J.: Description of Input and Examples for PHREEQC Version 3 — A Computer Program for Speciation, Batch-Reaction, One-Dimensional Transport, and Inverse Geochemical Calculations. *U.S. Geological Survey Techniques and Methods*, (2013), 497 p.

Trumpp, M., Ystroem, L.H., Kohl, T., Nitschke, F.: Creating a new database from a thermodynamic data compilation validated for scaling minerals in hydrothermal power plants for geochemical modeling in PHREEQC. In preparation.

Ystroem, L.H., Nitschke, F., Held, S., Kohl, T.: An Integrated Sensitivity Analysis for the Basalt Specific Multicomponent Geothermometer for high Temperature Settings. *Proceedings of World Geothermal Congress 2020+1*, (2021).

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