ALGAIAR, M. 2025. Improving geothermal resource assessment: a data-driven approach to chemical geothermometry using deep learning. Presented at the 2025 SEG (Society of Exploration Geophysicists) Net-zero emissions workshop, 23-25 June 2025, [virtual event].

# Improving geothermal resource assessment: a data-driven approach to chemical geothermometry using deep learning.

ALGAIAR, M.

2025

This output file contains the extended abstract and slides presented at the conference which have been incorporated into a single file.





# Improving Geothermal Resource Assessment: A Data-Driven Approach to Chemical Geothermometry Using Deep Learning

### Mahmoud AlGaiar

Robert Gordon University

### **Summary**

This study presents a deep learning model trained on a dataset of 674 water samples from Nevada to predict geothermal reservoir temperatures. The model outperforms traditional geothermometers and other machine learning models, achieving high accuracy and demonstrating global applicability when tested on samples from different geothermal fields around the world.

### Introduction

Geothermal energy is a promising source of renewable, clean and sustainable energy. Accurate prediction of subsurface temperatures is critical for geothermal and exploration development. Traditionally, this has been done using classical geothermometers, which rely on the chemical equilibrium between reservoir fluids and host rocks. However, these methods can be potentially unreliable due to factors such as fluid mixing and degassing. This study presents a novel data-driven model designed to overcome these limitations and provide more accurate temperature predictions for diverse geothermal systems.

The data-driven model harnesses the power of machine learning to analyze extensive hydrogeochemical data and identify patterns that may be missed by traditional methods. This innovative approach was trained and validated using a comprehensive dataset of 674 water samples from Nevada, a region known for its significant geothermal potential and diverse geological settings. The study also explores the geological and hydrogeological characteristics of Nevada's geothermal systems, examining factors such as fault systems, groundwater flow patterns, and water chemistry.

### Methodology

Recognizing the limitations of classical geothermometers and addressing the challenge of missing subsurface temperature measurements in the Nevada water sample dataset, subsurface temperature

was inferred using multiple techniques including classical and multicomponent geothermometry, regional thermal database extrapolation, and an existing machine learning geothermometer. This comprehensive approach ensured a robust dataset for training the machine learning model. After data preprocessing and exploratory data analysis, including feature selection and data clustering, the deep neural network model outperformed other machine learning models tested (Random Forest, XGBoost, and Back-Propagation Neural Network), achieving high accuracy  $(R^2 = 0.978)$  and low error rates on both the training and test datasets, as shown in Figure 1. Validation with 42 new well samples from different geothermal fields around the world confirmed its applicability and reliability in different geological environments.

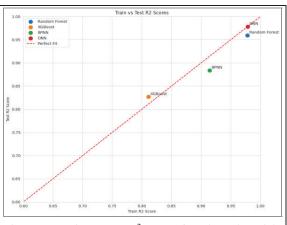


Figure 1: Train vs Test R<sup>2</sup> scores for adopted models

### Conclusions

This study successfully developed and validated a novel deep learning model for predicting geothermal reservoir temperatures using geochemical data. The model was trained on a comprehensive dataset of 674 water samples from Nevada, addressing the limitations of traditional geothermometers and leveraging the power of machine learning to identify complex patterns in hydrogeochemical data. The deep learning model outperformed other machine learning

### Improving Geothermal Resource Assessment: Geothermometry Using Deep Learning

models, including Random Forest, XGBoost, and Back-Propagation Neural Networks, achieving high accuracy ( $R^2 = 0.978$ ) and low error rates. The study addressed the challenge of missing subsurface temperature measurements in the dataset by employing a multi-pronged inference strategy that combined classical geothermometers, multicomponent geothermometry, regional thermal database extrapolation, and an existing machine learning geothermometer. This approach ensured a robust and reliable dataset for training and validation of the deep learning geothermometer. Furthermore, the global applicability of the model was demonstrated by testing it on 42 new well samples from different geothermal fields around the world, demonstrating its ability to perform well in different geological environments. This approach represents a significant advance in chemical geothermometry, providing a more accurate, efficient, and globally applicable tool for predicting subsurface temperatures geothermal exploration and reservoir characterization. Future research will focus on expanding the dataset, incorporating advanced feature engineering, and developing a user-friendly platform to disseminate the model's capabilities and further advance geothermal research and investment opportunities.

### Keywords

Geothermal Resource Exploration, Hidden/Blind Geothermal Resources, Artificial Intelligence, Machine Learning, Deep Learning

### Acknowledgements

The authors would like to acknowledge Robert Gordon University for providing resources and support for this paper and for their invaluable contributions to the completion of this research.

### References

Arnorsson, S., Sigurdsson, S. and Svavarsson, H., 1982.

The chemistry of geothermal waters in Iceland. I.
Calculation of aqueous speciation from 0 to 370
C. Geochimica et Cosmochimica Acta, 46(9),
pp.1513-1532. https://doi.org/10.1016/0016-7037(82)90311-8

# A Data-Driven Approach to Chemical

- Diaz-Gonzalez, L., Santoyo, E. and Reyes-Reyes, J., 2008.

  Three new improved Na/K geothermometers using computational and geochemiometrical tools: Application to the temperature prediction of geothermal systems. Revista mexicana de ciencias geológicas, 25(3), pp.465-482.
- Faulds, J.E., Coolbaugh, M.F. and Hinz, N.H., 2021. Inventory of Structural Setting for Active Geothermal Systems and Late Miocene (~ 8 MA) to Quaternary Epithermal Mineral Deposits in the Basin and Range Province of Nevada. Rep. - Nev. Bur. Mines Geol., 58, p. 28, 3 plates, scale 1:2,500,000.
- Faulds, J.E., Coolbaugh, M., Blewitt, G. and Henry, C.D., 2004. Why is Nevada in hot water? Structural controls and tectonic model of geothermal systems in the northwestern Great Basin. Geothermal Resources Council Transactions, 28, pp.649-654.
- Faulds, J. and Hinz, N., 2015, April. Favorable tectonic and structural settings of geothermal systems in the Great Basin region, western USA: Proxies for discovering blind geothermal systems. In Proceedings World Geothermal Congress, Melbourne, Australia, 19-25 April 2015 (No. DOE-UNR-06731-02). Nevada Bureau of Mines and Geology, University of Nevada, Reno.
- Fournier, R.O., 1979. A revised equation for the Na/K geothermometer. GRC Transactions, 3, pp.221-224.
- Fournier, R.O. and Truesdell, A.H., 1973. An Emprical Na-K-Ca Geothermometer for Natural Waters. Geochim. Cosmochim. Acta, 37, 1255-1275. https://doi.org/10.1016/0016-7037(73)90060-4
- Fournier, R.O. and Potter II, R.W., 1979. Magnesium correction to the Na-K-Ca chemical geothermometer. Geochimica et Cosmochimica Acta, 43(9), pp.1543-1550. https://doi.org/10.1016/0016-7037(79)90147-9
- Fournier, R.O., 1977. Chemical geothermometers and mixing models for geothermal systems. Geothermics, 5(1-4), pp.41-50. https://doi.org/10.1016/0375-6505(77)90007-4
- Freeze, R.A. and Cherry, J.A., 1979. Groundwater prentice-hall. Englewood Cliffs, NJ, 176, pp.161-177.
- Giggenbach, W.F., 1981. Geothermal mineral equilibria.

  Geochimica et Cosmochimica Acta, 45(3),
  pp.393-410. <a href="https://doi.org/10.1016/0016-7037(81)90248-9">https://doi.org/10.1016/0016-7037(81)90248-9</a>

# Improving Geothermal Resource Assessment: A Data-Driven Approach to Chemical Geothermometry Using Deep Learning

- Glassley, W.E., 2010. Geothermal energy: renewable energy and the environment (1st ed.). CRC press. <a href="https://doi.org/10.1201/EBK1420075700">https://doi.org/10.1201/EBK1420075700</a>
- Hodson, T.O., 2022. Root mean square error (RMSE) or mean absolute error (MAE): When to use them or not. Geoscientific Model Development Discussions, 2022, pp.1-10. https://doi.org/10.5194/gmd-15-5481-2022
- Lantz, B., 2019. Machine learning with R: expert techniques for predictive modelling. Packt publishing ltd.
- Maurer, D.K., Lopes, T.J., Medina, R.L. and Smith, J.L., 2004. Hydrogeology and hydrologic landscape regions of Nevada. USGS Scientific Investigations Report, 5131.
- Nevada Bureau of Mines and Geology (2022) Geothermal Minerals of Nevada. Available from https://storymaps.arcgis.com/stories/624b919af8c b4382824a47fd14fef13a. Accessed Sept 2024.
- Parkhurst, D.L. and Appelo, C.A.J., 2013. PHREEQC (Version 3)-A Computer Program for Speciation. Batch-Reaction, One-Dimensional Transport, and Inverse Geochemical Calculations. US Geological Survey, Water Resources Division, 6 (A43), 497. <a href="https://doi.org/10.3133/tm6A43">https://doi.org/10.3133/tm6A43</a>
- Piper, A.M., 1944. A graphic procedure in the geochemical interpretation of water analyses. Eos, Transactions American Geophysical Union, 25(6), pp.914-928. https://doi.org/10.1029/TR025i006p00914
- Siler, D.L., Faulds, J.E., Hinz, N.H., Dering, G.M., Edwards, J.H. and Mayhew, B., 2019. Three-dimensional geologic mapping to assess geothermal potential: examples from Nevada and Oregon. Geothermal Energy, 7, pp.1-32. https://doi.org/10.1186/s40517-018-0117-0
- Southern Methodist University (2024) Geothermal Laboratory Heat Flow Database. http://smu.edu/geothermal/. Accessed Sept 2023.
- Spycher, N., Peiffer, L., Sonnenthal, E.L., Saldi, G., Reed, M.H. and Kennedy, B.M., 2014. Integrated multicomponent solute geothermometry. Geothermics, 51, pp.113-123. <a href="https://doi.org/10.1016/j.geothermics.2013.10.01">https://doi.org/10.1016/j.geothermics.2013.10.01</a>
- Tut Haklidir, F.S. and Haklidir, M., 2020. Prediction of reservoir temperatures using hydrogeochemical data, Western Anatolia geothermal systems (Turkey): a machine learning approach. Natural

- Resources Research, 29(4), pp.2333-2346. https://doi.org/10.1007/s11053-019-09596-0
- University of Nevada: Geothermal Energy. https://nbmg.unr.edu/Research/GeothermalEnerg y.html (2024). Accessed 25 Sept 2024.
- Ystroem, L.H., Vollmer, M., Kohl, T. and Nitschke, F., 2023. AnnRG-An artificial neural network solute geothermometer. Applied Computing and Geosciences, 20, p.100144. https://doi.org/10.1016/j.acags.2023.100144



# **Geothermal Overview**

1

# **Renewable Source**

Geothermal energy is derived from Earth's heat, providing stable, sustainable power.

2

# **Global Growth**

Geothermal energy could meet 15% of global electricity demand by 2050, with a potential potential global capacity of 800 gigawatts - equivalent to the current electricity demand of the demand of the US and India combined (IEA 2025).

3

# **Key Countries**

Significant in USA, Indonesia, Philippines, Türkiye, and New Zealand.

# **Exploration Challenges**

1 \_\_\_ Financial Risks

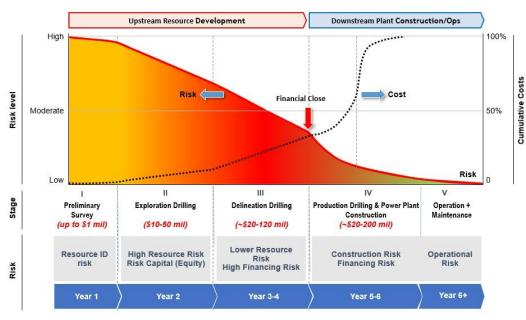
High costs during predevelopment stages, including surface surveys and exploratory drilling.

Hidden Resources

Difficulty in identifying blind geothermal resources without surface manifestations.

Expert Reliance

Traditional methods heavily depend on expert expert knowledge, leading to uncertainties. uncertainties.



The stages of the geothermal development project and its risk levels (Gehringer and Loksha, 2012).



# **Geochemical Analysis**

# **Cost-Effective**

Geochemical data from groundwater samples are crucial in early exploration stages.

# Insightful

Provides valuable information on subsurface characteristics and reservoir properties.

# **Analytical**

Helps determine reservoir temperature, heat flow, and potential for energy extraction.



# Geothermometry

1

# **Classical Geothermometers**

function based on temperature-dependent mineral-fluid equilibrium reactions, primarily utilizing silica concentrations and cation ratios (Na-K, Na-K-Ca, K-Mg) in geothermal waters.

2

# **Multicomponent Geothermometry**

analyzes the equilibrium between multiple minerals, focusing on the convergence of mineral saturation indices at the true reservoir temperature.

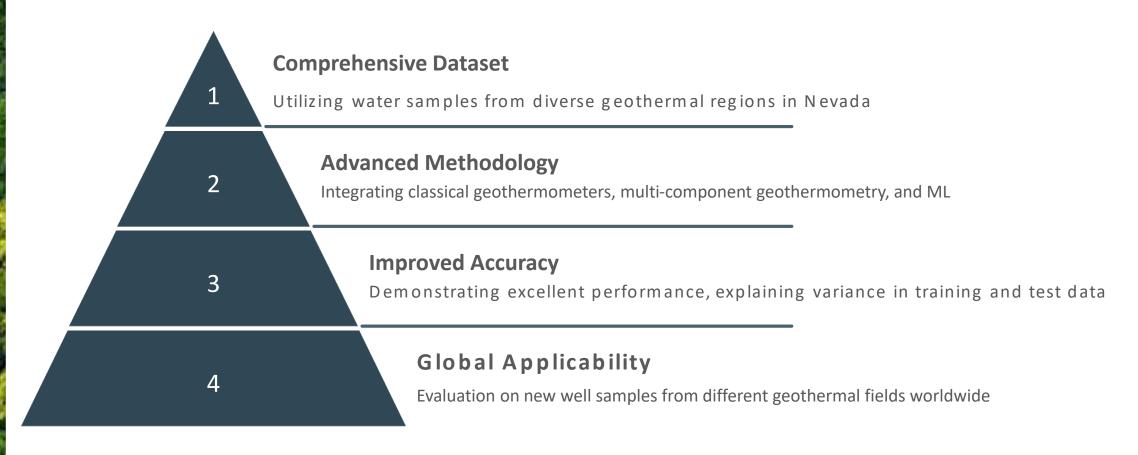
3

# **Data-Driven Geothermometers**

a modern approach that utilizes machine learning and statistical methods to establish correlations between fluid chemistry and reservoir temperatures.



# Methodology





# **Exploratory Data Analysis**

1

### **Extensive Dataset**

Analysis of over 14,400 geochemical samples from the Great Basin Groundwater Groundwater Geochemical Database. This vast collection of information forms the forms the backbone of the platform's predictive capabilities.

2

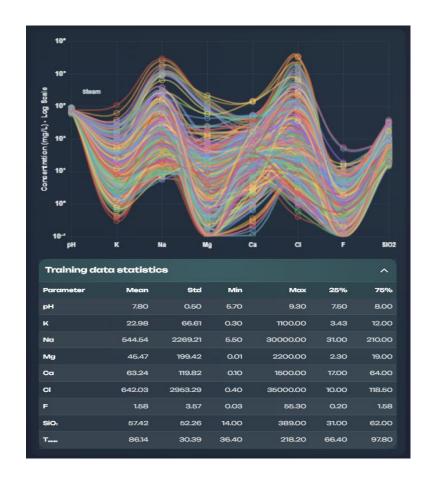
# **Data Integrity**

To ensure data quality, the model performs a charge balance error calculation, rejecting samples outside the acceptable range of  $\pm 5\%$ . This rigorous approach guarantees the reliability of the input data.

3

### **Feature Selection**

Through exploratory data analysis, eight key features were identified as strong strong influencers of temperature: **potassium**, **sodium**, **magnesium**, **calcium**, **calcium**, **calcium**, **chloride**, **fluorine**, **silica**, and **pH**. These elements form the core of ailON's of ailON's predictive model.





# **Data Processing**

Data Transformation

Employing various data transformation methods, including z-score, logarithmic transformation, and quantile normalization. These techniques optimize model performance and ensure accurate predictions.

**Clustering Analysis** 

Utilized clustering techniques such as K-as K-means and Hierarchical Clustering Clustering to identify patterns within within the dataset. This approach helps helps in understanding the underlying underlying structure of the geochemical geochemical data.

**ML Model Development** 

Several machine learning algorithms were evaluated to determine each algorithm's algorithm's predictive ability and to determine the best model.

Random Forest (RF) Ensemble learning method using multiple decision trees **Gradient Boosting (XGB)** Builds new trees sequentially to reduce bias from previous trees **Artificial Neural Network (ANN)** Simple backpropagation neural network with four layers **Deep Neural Network (DNN)** More complex architecture with three three hidden layers and advanced techniques



# **DNN Model Performance Metrics**

0.9784

DNN R<sup>2</sup> (Train)

Coefficient of determination for training data

4.0097

**DNN RMSE** 

Root Mean Square Error for test data

0.9783

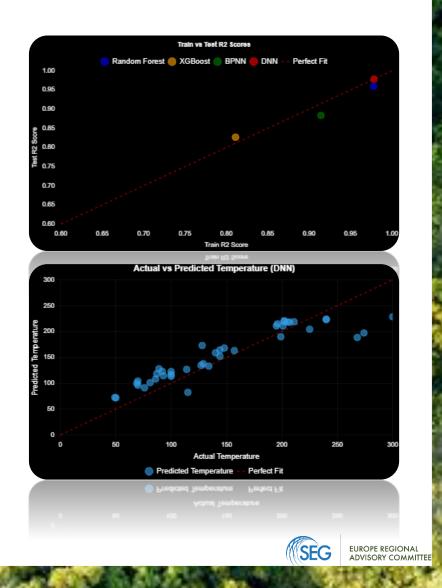
DNN R<sup>2</sup> (Test)

Coefficient of determination for test data

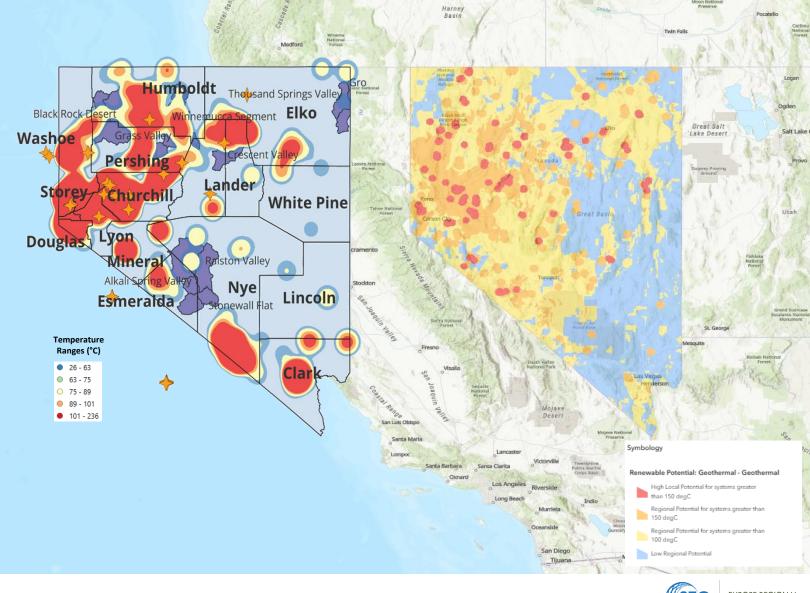
2.6363

**DNN MAE** 

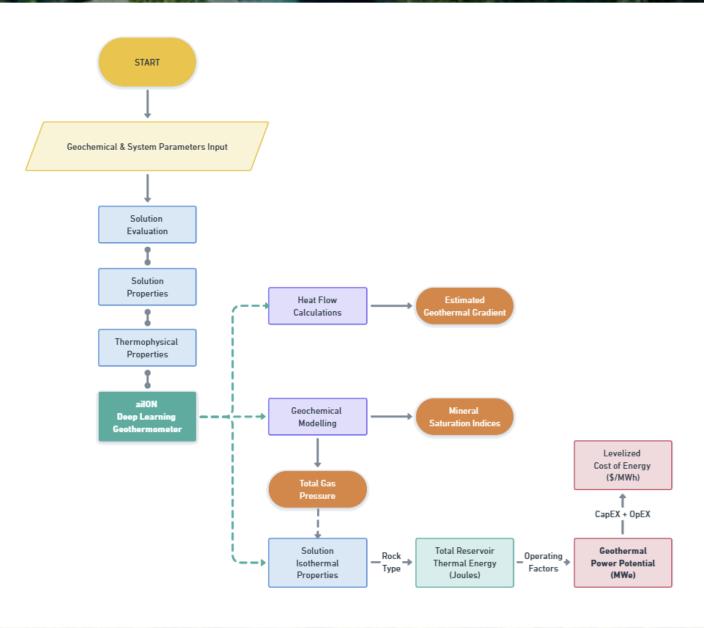
Mean Absolute Error for test data



# Nevada Geothermal Potential Map



# ailON Software Platform





# **Solution Properties Module**

Classification

Categorize water based on its properties, properties, including **class**, **type**, and and **description**. This classification helps helps in understanding the nature and and origin of the geothermal fluid.

Hydrogeochemical Processes

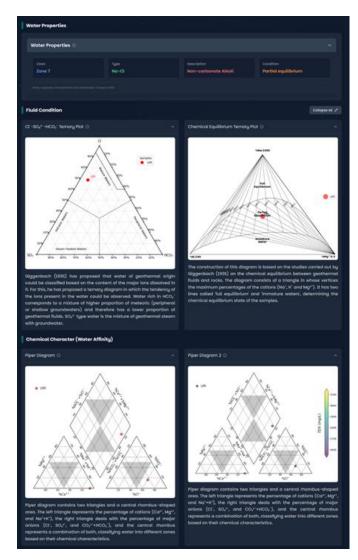
Understanding the mechanisms controlling water chemistry. It helps helps identify the dominant processes processes affecting the geothermal geothermal fluid composition and controlling water chemistry and rock rock weathering, categorizing samples samples into precipitation-dominated, dominated, rock weathering-dominated, and evaporation/crystallization-controlled types.

Chemical Equilibrium State

Determine the chemical equilibrium state of the water, providing insights into its **maturity** and potential for geothermal energy production.

Trace Elements Analysis

Ternary Diagrams to visualize the relationships between Cl<sup>-</sup>, B, and F<sup>-</sup> F<sup>-</sup> concentrations and Cl<sup>-</sup>, B, and Li<sup>+</sup> Li<sup>+</sup> concentrations in the geothermal geothermal fluid. This analysis helps in helps in understanding the fluid's origin origin and evolution.





# **Geochemical Modelling Module**

### **Molality and Moles**

Lists the molality and moles of various elements, including C, Ca, Cl, F, K, Mg, Na, S, and Si.

# **Solution Description**

Provides detailed information including Sample ID, pH, pe, Activity of water, Ionic strength, Mass of water, Total alkalinity, Total CO<sub>2</sub>, and Electrical balance.

## **Species Distribution**

Lists the molality, activity, and log activity of various species, such as  $OH^-$ ,  $H^+$ ,  $H_2O$ ,  $HCO_3^-$ ,  $Ca^{2+}$ ,  $CI^-$ ,  $F^-$ ,  $K^+$ ,  $Mg^{2+}$ ,  $Na^+$ ,  $SO_4^{2-}$ , and  $SiO_2$ .

# **Mineral Saturation Analysis**

This module provides a comprehensive comprehensive summary of mineral saturation indices, indicating the extent of extent of their saturation in the geothermal geothermal fluid. This information is crucial crucial for understanding the chemical chemical equilibrium of the system.

### **Gas Fugacity and Pressure**

ailON calculates and reports the fugacity and partial pressure of gases in the solution, such as  $CO_2$  and  $H_2O$ . This data is essential for understanding the behavior of gases in the geothermal reservoir.





# **Thermophysical Module**

1

2

3

# **Comprehensive Solution Properties**

ailON calculates crucial thermophysical properties including solution quality, density, specific volume, dynamic viscosity, thermal conductivity, internal energy, entropy, enthalpy, and heat capacity.

# **Geothermal Gradient Analysis**

Computing effective thermal conductivity and geothermal gradients, providing insights into the heat distribution within the reservoir.

# **Heat Flow Assessment**

ailON calculates heat flow, a critical parameter for understanding the energy potential of a geothermal system.





# **Geothermal Potential Module**



# **Thermal Energy Calculation**

Computes total thermal energy of the reservoir



### **Power Potential Estimation**

Calculates potential power output in Watts and MWe



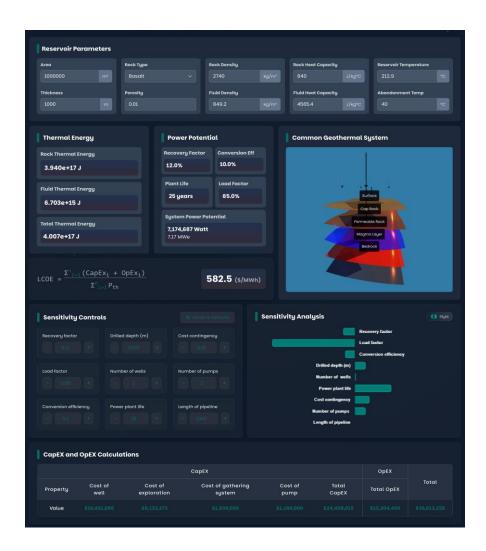
# **Economic Viability Analysis**

Calculation of CapEX & OpEX and determining the LCOE



# **Sensitivity Analysis**

Allows adjustment of key parameters for scenario planning





# Implications for Geothermal Exploration

1

# **Improved Accuracy**

ailON provides reliable temperature predictions for geothermal reservoirs

2

# **Cost-Effective Exploration**

Reduces the need for expensive drilling and testing in early exploration stages

3

# **Blind System Identification**

Enhances ability to locate and assess "blind" geothermal systems without surface manifestations

4

### **Resource Assessment**

Facilitates more accurate estimation of geothermal potential in unexplored areas









Mahmoud M. AlGaiar



m.algaiar@rgu.ac.uk



+966 50 929 4686









# Research Supervisory Team

Prof. Nadimul Faisal<sup>a</sup>, Dr. Shahana Bano<sup>a</sup>, Prof. Mamdud Hossain<sup>a</sup>, Prof. Aref Lashin<sup>b</sup>, Dr. Hend S. Abu Salem<sup>c</sup>

<sup>a</sup>School of Computing, Engineering and Technology, Robert Gordon University, Garthdee Road, Aberdeen, AB10 7GJ, UK <sup>b</sup>Petroleum and Natural Gas Engineering Department, College of Engineering, King Saud University, Riyadh, Saudi Arabia <sup>c</sup>Geology Department, Faculty of Science, Cairo University, Giza, 12613, Egypt

