Lithium Estimation AI Tool: Overview, Technologies, and Value

The **Lithium Estimation AI Tool**, developed by INLECOM within the Horizon Europe CRM-Geothermal project, represents a pioneering approach to leveraging Artificial Intelligence (AI) for optimizing lithium exploration in geothermal resources. At a time when the global demand for lithium is rapidly increasing due to its vital role in battery technologies and renewable energy storage, this tool offers a unique solution to support sustainable raw material supply chains.

Functional Overview

The CRM AI Tool comprises **two core functionalities** designed to address different analytical needs:

1. Feature Importance and Interpretability

In this mode, users can either input custom sample data or select existing records from the CRM dataset. The tool estimates lithium concentration and provides a comprehensive interpretability interface. A **Waterfall Shapley plot** shows how each element increases or decreases the predicted lithium level relative to the dataset average. Users can trace how the decision tree navigated through feature splits, visualizing how the model progressively refined the prediction. Additionally, scatterplots illustrate the relationships between lithium and each elemental concentration, and a geospatial map situates the sample within the broader reservoir landscape. This combination empowers users to validate predictions, explore analogs in the data, and detect potential outliers.

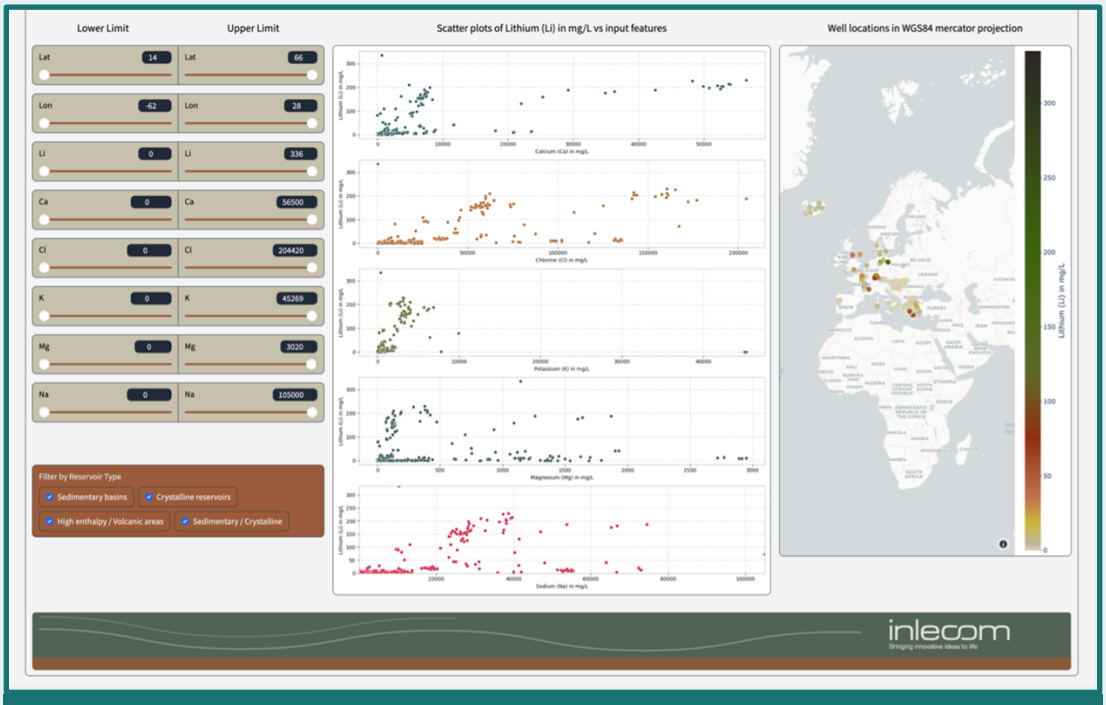

Figure 1: Interpretability in Data Clusters- Sliders, Reservoir filter, Scatterplots and map.

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2. Feature Relationships and Geographic Patterns

The second functionality enables exploratory data analysis across the entire dataset or filtered subsets. Users can define value ranges for input features, select specific reservoir types, and instantly retrain a decision tree model tailored to these constraints. The resulting **Beeswarm Shapley plots** and performance metrics help users assess how the importance of variables shifts within different geological or chemical contexts. This mode is particularly valuable for identifying trends, such as regional hotspots of lithium enrichment or correlations unique to certain reservoir types.

The tool positions INLECOM at the forefront of AI-enabled mineral exploration. Its **high value proposition** lies in three core benefits for target audiences:

- **Enhanced Exploration Efficiency:** By integrating geochemical data interpretation into a transparent, user-friendly AI platform, the tool reduces time and resources required to evaluate lithium potential in geothermal wells.
- **Actionable Insights for Decision Making:** Through its explainable model outputs, the tool enables stakeholders to justify investment and policy decisions with clear evidence of the geochemical drivers of lithium occurrence.
- **Sustainability and Strategic Autonomy:** As Europe intensifies efforts to secure critical raw materials sustainably, this AI solution supports regional self-sufficiency by optimizing domestic geothermal resources.

The Value of AI in Lithium Exploration

The incorporation of AI into geothermal lithium exploration delivers transformative advantages over traditional analytical approaches. While conventional statistical models are constrained by assumptions of linearity and homogeneity, AI methods—particularly tree-based ensemble approaches—can naturally capture **non-linear dependencies, complex interactions among variables, and hidden patterns in large datasets**. This ability to model subtle and often counterintuitive relationships is crucial in geothermal systems, where elemental concentrations are governed by intertwined geological, chemical, and thermal processes.

Beyond predictive accuracy, AI provides unprecedented **scalability**: the same model can be retrained or fine-tuned to accommodate new data sources, extended feature sets, or different reservoir types. This adaptability ensures that as new geothermal wells are explored and more measurements become available, the CRM AI Tool remains a relevant and evolving asset.

Equally important is the emphasis on **explainability**, which transforms AI from a “black box” into a transparent decision support system. By quantifying each feature’s contribution to a prediction, the tool fosters confidence among stakeholders and supports defensible decisions about exploration investments and resource management. In regulatory or commercial contexts, this transparency is increasingly vital.

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Technical Developments

The tool's development was structured through a comprehensive process that combined **geological expertise**, **data science**, and **explainable machine learning** techniques. From the outset, INLECOM set out to address a key challenge: understanding the complex and often non-linear relationships between dissolved elements in geothermal fluids and lithium concentrations. The initial phase involved refining and cleaning extensive geothermal datasets. In particular, the **REFLECT dataset** was transformed into an upgraded CRM-geothermal database. This step ensured a robust foundation for AI model development by correcting inconsistencies such as misplaced decimal values, erroneous or missing coordinates, and incomplete records. **Data engineering** played a pivotal role in preparing the dataset for advanced analysis. The team developed a **bespoke methodology** for outlier detection and data augmentation. For example, where individual wells had limited samples, synthetic samples were generated to ensure balanced representation across wells, thereby minimizing bias in model training. Equally important was the **imputation strategy**, which maintained the variability of wells while filling gaps in data without distorting the underlying distributions.

Following extensive statistical exploration, conventional linear models were found inadequate to capture the intricate dependencies among elements such as magnesium (Mg), potassium (K), sodium (Na), calcium (Ca), and chlorine (Cl). As a result, the team adopted **Decision Tree Regression**, a machine learning approach well-suited to modeling non-linear relationships and providing transparent interpretability. The Decision Tree model achieved commendable predictive performance, with a **Root Mean Squared Error (RMSE) of 9.74 mg/L**, highlighting its reliability in estimating lithium concentrations from multivariate elemental data.

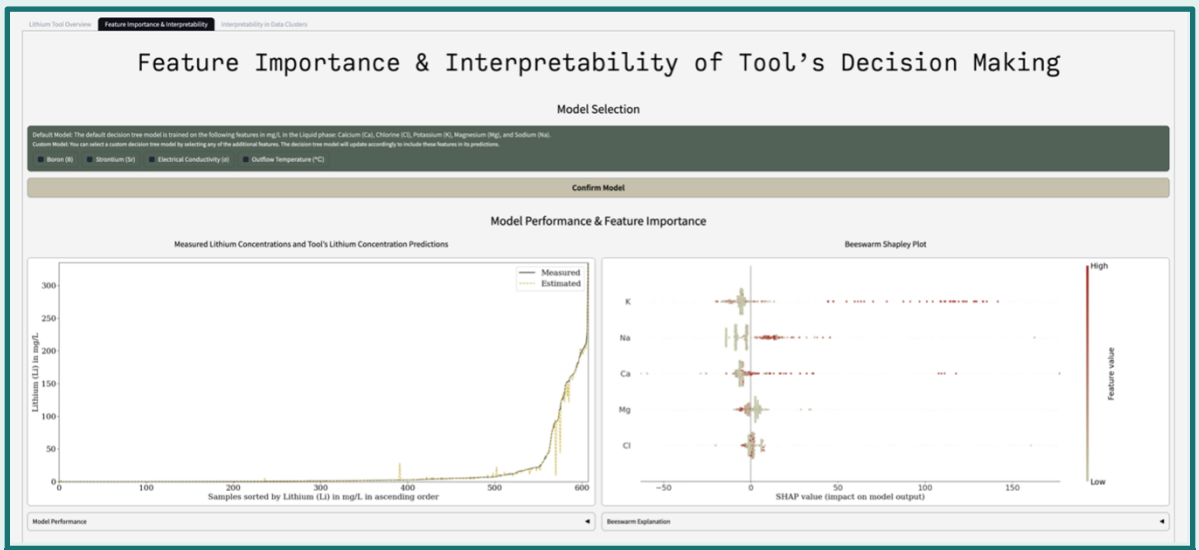

Figure 2: Model selection, model performance and feature importance.

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A distinguishing feature of the CRM AI Tool is its commitment to **Explainable AI**. Recognizing that end users—geoscientists, resource managers, and policymakers—require not only predictions but also clarity about how those predictions are derived, the project integrated **Shapley values** to interpret model outputs. Shapley values decompose each prediction to show the individual contribution of each input variable, offering actionable insights into which elemental features drive lithium enrichment in specific geothermal contexts. For instance, potassium emerged as the most influential predictor in many scenarios, though its effect was non-linear and context-dependent, underscoring the complexity of geothermal geochemistry.

Feedback collected from consortium partners via structured questionnaires was used to fine-tune the tool's interface and analytical capabilities, ensuring alignment with real-world needs. The final release includes comprehensive documentation and an intuitive interface accessible to both technical and non-technical users.

In conclusion, the **Lithium Estimation AI Tool** stands as a concrete example of how **AI and data-driven methodologies can transform critical raw material exploration**, combining scientific rigor with practical usability. It demonstrates how digital solutions can help Europe and the global community advance towards a more sustainable, resilient, and strategically autonomous energy future.

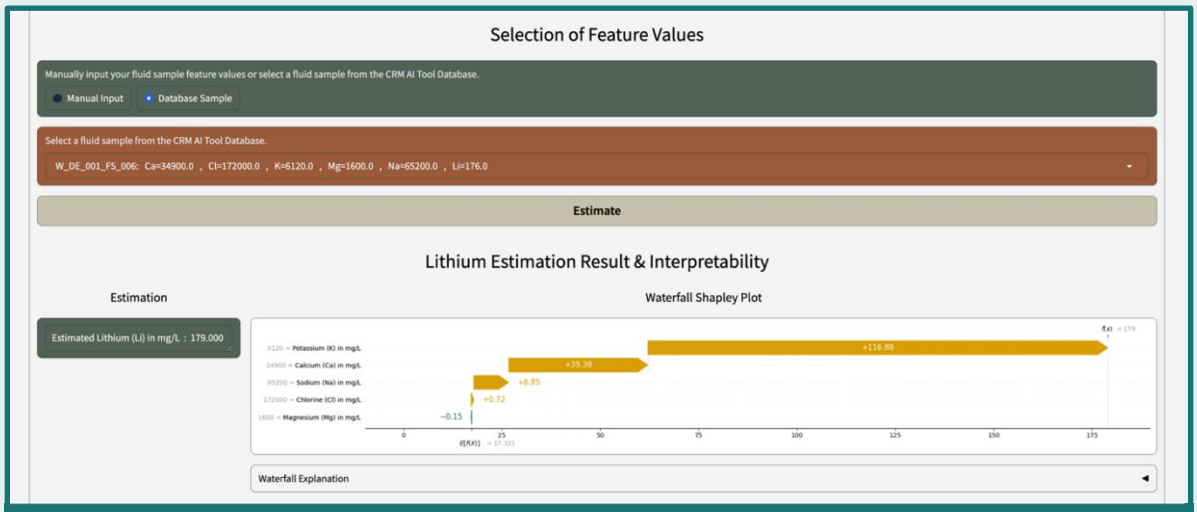

Figure 3: Lithium Estimation and results Interpretation.

Access the AI Tool: https://crm.inlecom.eu/

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