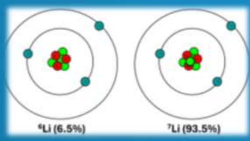
A first approach to the development of formulations for lithium isotope enrichment for Fusion by liquid extraction with complexing agents using machine learning techniques

Annalisa Congiu[1], Roberto Simone Pinna[2], Riccardo Po'[1] and Giacomo Melani[1]
[1]Renewable, New Energies and Material Science Research Center and R&D Business Partner, Eni S.p.A., via Fauser 4, Novara, Italy
[2]Data, AI & Agile Experience Center of Excellence, Eni SpA, San Donato Milanese, Italy
annalisa.congiu@eni.com



Introduction

Eni's research is committed to developing fusion energy production as part of its energy transition initiatives. The basis of the technology is the fusion reaction between two hydrogen nuclei, deuterium and tritium:

$D + T \rightarrow {}^4_2He + n + 17{,}6\ MeV$

Tritium is a ß radiator and only exists in nature in negligible quantities. Tritium must therefore be produced in situ. The most suitable material for producing tritium is lithium. Lithium exists in nature in the form of two isotopes: ^{7}Li with an abundance of 92.5% and ^{6}Li with an abundance of 7.5%. Both can produce tritium by neutron bombardment according to the reactions:

$${}^6_3Li + {}^1_0n \rightarrow {}^3_1T + {}^4_2He + 4{,}8\ MeV$$
$${}^7_3Li + {}^1_0n \rightarrow {}^3_1T + {}^4_2He + n' - 2{,}466\ MeV$$

The reaction of ^{6}Li is exothermic and contributes significantly to the energetic output of the fusion reactor, whereas the reaction of ^{7}Li is endothermic and results in a loss of energy. Moreover, the cross section of the ^{6}Li is much larger than that of the ^{7}Li, especially for thermal neutrons. For the energy balance to be favorable, the ratio of tritium production to consumption must be sufficiently greater than 1 (Tritium Breeding Rate TBR>1). To achieve this with an energy balance suitable for sustaining the plasma and the fusion reaction, the lithium must be enriched in a 6-mass component.
The level of enrichment depends on the reactor design and in particular the blanket-concept and is estimated at between 30% and 90%.

HCPB (Helium Cooled Pebble Bed)
- Li_4SiO_4 or Li_2TiO_3
- ^{6}Li enrichment: 40-60%

HCLL (Helium Cooled Lithium Lead)
- eutectic LiPb
- ^{6}Li enrichment: >90%

Liquid Immersion Blanket
Molten Salt (FLiBe)
^{6}Li enrichment: tbd

Main technologies for isotopic enrichment of ^{6}Li

1. Chemical exchange methods:
   - lithium amalgam system
   - liquid ammonia system
   - cation complexing systems using mainly cyclic polyethers and cryptands (liq-liq extraction)
   - intercalation systems
   - organic or inorganic ion exchangers (displacement chromatography methods)
     - Ion-Exchange Resins Ion-exchange
     - Resin-Supported Complexing Agents
     - Ion-Exchange Membrane

   → CHEMICAL EXCHANGE

2. Electrochemical exchange methods
   - electrolyses on mercury or other cathodes
   - electromigration
   - electrophoreses
   - diffusion and electromigration

   → ELECTROCHEMICAL EXCHANGE

3. Laser methods LIS
   - Atomic Vapour LIS
   - MLIS – Molecular LIS

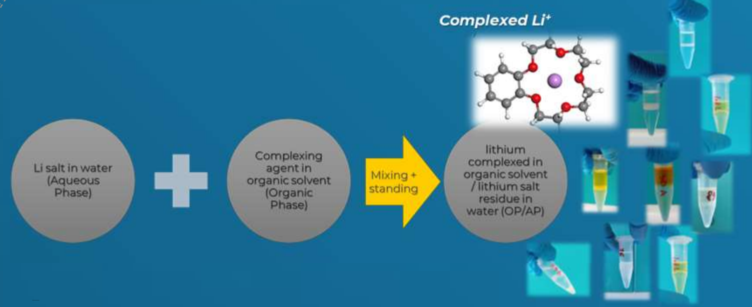
   → LASER TECHNOLOGY

4. Thermal Diffusion
5. Distillation
6. Fractional Cristallization
7. Radiofrequency Spectroscopy
8. Microalgal Enrichment Process
9. Centrifuge exctraction

   → OTHERS

...and combinations of these technologies

Cation complexing systems – liquid –liquid extraction



The formulation involves combining many parameters that must generate systems that are easily miscible, with optimal solubility for the complexing agent and rapid chemical exchange.

Enrichment factor
$\alpha = (^6Li/^7Li)_{OP} / (^6Li/^7Li)_{AP}$

Distribution factor
$D = [Li]_{OP}/[Li]_{AP}$

Hybrid Database: A Foundation for Data-Driven Extraction Process Development

Our approach integrates diverse information into a **hybrid database**, comprising literature , experimental and material data.

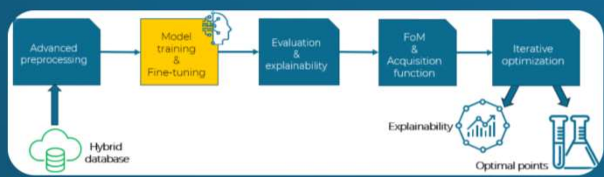
- **Systematic Data Extraction:** we built a dedicated extraction database by extracting and standardizing data from relevant literature. This involved defining a robust data model and implementing a rigorous preprocessing pipeline to unify disparate units and boundary conditions, and manage sparse, categorical data through custom imputation.
- **Chemical Property Integration:** to enhance data effectiveness, we created a parallel database of chemical substances (salts, complexants, solvents and co-solvents) and their relevant physicochemical properties. This innovative step allows us to replace categorical chemical names with quantifiable features.
- **Dynamic Data Enrichment & Dimensionality Reduction:** The hybrid database is fed to a dimensionality reduction pipelines (e.g., PCA) to manage the increased complexity and prepare the data for effective machine learning analysis.

This hybrid database structure provides a robust, standardized, and information-rich foundation, enabling the application of advanced machine learning techniques for extraction process optimization.

Optimal Experimental Design with AI

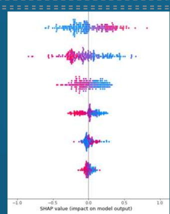
A tailored Machine Learning (ML) pipeline has been designed to learn complex relationships within the hybrid database and propose optimal experimental conditions. This tool streamlines the discovery process and minimizes resource-intensive experimentation.

1. **Smart Preprocessing:** ensures data quality and prepares it for model training. Key steps include cleaning low-informative data, outlier detection, intelligent missing data imputation with ML and dimensionality reduction.
2. **Adaptive Proxy Modeling:** we develop highly accurate ML models to predict target variables (e.g. α, D) from experimental parameters. It implements hyperparameter tuning for smart imputation and proxy model, it features also a comprehensive performance evaluation and agnostic evaluation by Predictive Power Score (PPS).
3. **Intelligent Optimization & Experimental Design**
   - **Custom Figure of Merit (FoM):** tailored target function to allow quantitative comparison and optimization across multiple target values, reflecting real-world experimental objectives.
   - **Acquisition Function:** it combines the model's predictions, predictive uncertainty and a learned empirical error, estimated by training an ML model dedicated to leave-one-out errors.
   - **Iterative optimization algorithms:** the acquisition function is incorporated into genetic optimization algorithms to explore the experimental domain and identify new points by balancing the pursuit of target values with the need to reduce domain uncertainty.



Shapley explainability

We leverage Shapley values to provide transparent and actionable insights into our proxy models. Rooted in cooperative game theory, offer a robust and theoretically sound method for attributing the contribution of each input feature to the model's predictions.
Global Feature Impact: quantifies the average influence of each input feature on model predictions, highlighting key variables.
Directional Influence: indicates whether a feature tends to increase or decrease the predicted target.
Scientific Validation: helps verify model consistency with physical phenomena and uncover novel dependencies.
This interpretability layer transforms our predictive models into more transparent tools, fostering deeper scientific understanding and accelerating decision-making in Lithium-6 extraction development.



Conclusion

This project establishes a comprehensive, data-driven framework for optimizing Lithium-6 isotope enrichment via liquid-liquid extraction.
Integrated ML Framework: We developed and trained a customizable ML model, leveraging both literature and experimental data, for predicting and optimizing extraction efficiency. This framework includes a user-friendly interface for data analysis, model management, and result visualization.
Intelligent Experimentation: The model effectively suggests trial parameters and predicts key performance indicators (enrichment factors α, extraction efficiency D, custom FoM). While currently showing an approximate 30% error, this provides actionable guidance for R&D and indicates areas for future model refinement through new data.
Global interpretation: via explainability techniques, we revealed critical information about the influence of the parameters considered. We validated consistency with physical phenomenology, identifying key dependencies that align with experimental findings.
Path Forward: the current prototype highlights the fundamental role of the quality and quantity of data contained in the database. Continuous expansion of the database, particularly in areas characterized by experimental heterogeneity, is essential to improve predictive accuracy and fully exploit the potential of the ML model to optimize the development of formulations for lithium-6 enrichment through liquid-liquid extraction.

References

1. *Giegerich T., Report on the assessment of a viable route for the separation of lithium isotopes, internal report TRANSversal Actions for Tritium, KIT, 2019*
2. *Murali, A., Zhang, Z., Free, M. L., Sarswat, P. K., A Comprehensive Review of Selected Major Categories of Lithium Isotope Separation Techniques, Phys. Status Solidi A, 2100340 (2021) 1-21*
3. *Symons, E. A., Lithium Isotope Separation: A Review of Possible Techniques, Separation Science and Technology, 20 9-10, (1985) 633-651*
4. *Ault, T, Brozek, K., Fan, L., Folsom M., Kim, J, Zeismer, J., Lithium Isotope Enrichment: Feasible Domestic Enrichment Alternatives, Report UCBTH-12-005, Department of Nuclear Engineering University of California, Berkeley, 2012*
5. *Badea, S. L., Niculescu, V. C., & Iordache, A. M., New Trends in Separation Techniques of Lithium Isotopes: A Review of Chemical Separation Methods. Materials, 16 3817 (2023) 1-15*
6. *He, P, Xie Q., Wang J., Yao G., Wang L., Progress and Perspective of Lithium Isotope Separation, ChemPhysChem, 26 (2025) 202400999*
7. *Nishizawa, K, Takano, T. Ikeda, I., Okohara M., Extractive Separation of Lithium Isotopes by Crown Ethers Separation Science and Technology, 23 4-5 (1988) 333-345*
8. *Pei, H. Yan, F., Liu, H. He, B. Li, J., The selective complexation of crown ethers for lithium isotope separation: A critical review, Separation and Purification Technology 341 126857 (2024) 1-13*
9. *Segantin, S., Testoni, R., & Zucchetti, M. (2020). Neutronic comparison of liquid breeders for ARC-like reactor blankets. Fusion Engineering and Design, 160(2020), 112013.*