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A First Approach to the Development of Formulations for Lithium Isotope Enrichment for Fusion by Liquid Extraction with Complexing Agents Using Machine Learning Techniques

One of the crucial aspects in the development and commercialization of D-T fusion is the feeding of Tritium, which requires mass-enriched lithium 6, a minority isotope in nature (about 7%).
Although chemical properties are directly related to the electronic configuration of the atom, the mass difference between the isotope nuclei confer slightly different behavior to molecules and ions containing different isotopes of the same element and termed isotopologues. This phenomenon is known as the isotope effect and has been observed in a multiplicity of ways that have inspired the proposal of many technologies for isotopic separation [1-5]. The realization of a process for lithium isotope enrichment is complex and energy intensive because of the high number of stages required to achieve the targets and estimated quantities needed for fusion reactors currently under consideration. Except for mercury amalgam exchange technology (COLEX process, developed for military purposes in the 1960s and therefore still classified) possible technologies have very low TRLs and little information is disclosed about their potential development.
One of the most studied technologies is liquid-liquid extraction with complexing agents on which a substantial literature exists since the 1980s [6-7]. Isotopic enrichment occurs by complexation and extraction from lithium salts dissolved in water. Rationalization of the many parameters that impact equilibria is complicated by the fragmented nature of the sources. This presentation illustrates the creation of a PoC of a Machine Learning model capable of supporting experimentation through design of experiment.
The activity performed concerns:
• development of an Extraction Process Database and its Analysis
• implementation and optimization of Machine Learning (ML) pipeline
• development of an explainability process to uncover the relations between variables and target values;
• development of a user interface

Development and critical points of this approach are discussed.

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