**Toward Optimized Ligand Selection: A Review for Nuclear Fuel Reprocessing**

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# Abstract

Aqueous reprocessing of used nuclear fuel (UNF) is essential for reducing its long-term radiotoxicity and enhancing the safety and public perception of nuclear energy. Traditional aqueous reprocessing R&D involves testing the extraction efficiency of proposed ligand scaffolds with iterative ligand design and system condition changes. However, this laborious approach, coupled with the iterative nature of ligand development, significantly limits progress in nuclear separation technologies. Traditional approaches to ligand design often rely on incremental modifications of familiar molecular families, overlooking key factors like radiolytic resistance and process scalability, which are pivotal for industrial applications. Our literature review aims to evaluate critical data and process parameters essential for selecting ligands in the nuclear fuel cycle, with the goal of identifying strategies to enhance separation processes for lanthanides, actinides, and other valuable elements. The ligand selection criteria are categorized into three groups: chemical, process, and physical parameters, ranked by importance, to streamline their prioritization in ligand design pipelines. The potential for innovative ligand design to address critical challenges in nuclear waste management, such as improving efficiency, reducing process stages, and enhancing long-term sustainability, is highlighted in this review. Our research advances ligand discovery insights, providing a framework to expedite cutting-edge reprocessing technologies and foster innovation in nuclear waste management.

# Keywords

*Ligand selection; nuclear reprocessing; aqueous nuclear separations; nuclear waste management; f-block elements*

# Introduction

# Classification of Parameters

# Chemical Parameters – High Importance

# Process Parameters – Medium Importance

# Physical Parameters – Low Importance

# Discussion

## Summary of Critical Data and Process Parameters

## Implications for Nuclear Fuel Reprocessing

## Future Directions

# References