PHD PROJECT DESCRIPTION

(4000 characters max., including the aims and work plan to de published online)

Project title:

Molecular mechanisms of transport and selectivity in green polymer inclusion membranes modified with natural deep eutectic solvents (NADES) for critical metal recovery.

1.1. Project goals

Chemometric design and synthesis of innovative hydrophobic NADES characterized by high affinity for strategic metal ions and compatibility with the polymer matrix.

Evaluation of NADES as multifunctional components in polymer inclusion membranes (PIMs) to eliminate the need for synthetic, toxic plasticizers.

Optimization of "Green-PIMs" composition for the selective recovery of critical raw materials (In, Co, Li, etc.)

Elucidation of molecular transport mechanisms by determining the physicochemical parameters (diffusion coefficients, activation energy) and the role of hydrogen bond networks in ion/molecule recognition.

Assessment of membrane structural integrity and resistance to component leaching during long-term operational processes.

Development of an advanced mathematical and predictive QSPR model to correlate NADES molecular structure with transport efficiency and selectivity.

1.2. Outline

Nowadays, the recovery of strategic metals such as indium, cobalt, nickel etc. from secondary resources is a global priority due to their critical role in modern technologies and limited substitutability. Membrane techniques, particularly PIMs, offer a versatile platform for these challenges.

A breakthrough direction in membrane science is the integration of NADES as functional carriers or plasticizers. NADES, composed of primary metabolites (e.g., terpenes, organic acids, or choline derivatives), represent a "green" alternative to traditional, often toxic, organophosphorus extractants and ammonium salts. These solvents exhibit unique properties such as negligible vapor pressure, non-flammability, and high thermal stability.

The core scientific advantage of NADES lies in their molecular tunability. By careful selection of hydrogen bond donors and acceptors, it is possible to design hydrophobic NADES that remain stable in aqueous environments, effectively preventing the leaching of membrane components—a major drawback of classical PIMs. Therefore, this project proposes application of NADES-doped membranes for selective recovery high-purity metals from e-waste and electroplating wastewater.

1.3. Work plan

Molecular design and synthesis: Selection of natural precursors and synthesis of hydrophobic NADES; characterization of their physicochemical properties (density, viscosity, logP).

Membrane fabrication: Preparation of PIMs using various polymer matrices (e.g., CTA, PVC, etc.) and optimized NADES concentrations to achieve a balance between stability and flux.

Advanced morphological and interfacial study: Comprehensive analysis using AFM (surface roughness), SEM-EDX (elemental mapping), and FT-IR/NMR spectroscopy to understand the interactions between NADES, the polymer matrix, and the target substance.

Process optimization by chemometrics: Utilization of response surface methodology (RSM) to maximize selectivity and efficiency.

Kinetic modeling: Derivation of a mathematical model describing the transport process, including the determination of limiting steps (diffusion vs. chemical reaction).

Validation: Testing the optimized "Green-PIMs" for the separation of metals from complex industrial solutions.

1.4. Literature (max. 7 listed as a suggestion for a PhD candidate preliminary study)

Dwamena, A. K. (2019). Recent Advances in Hydrophobic Deep Eutectic Solvents for Extraction. *Separations*, *6*(1), 9. 10.3390/separations6010009
A. Falahudin, N. Insin, M. M. Khan, Hydrophobic Deep Eutectic Solvents: Synthesis, Properties, Applications, and Future Directions, *Journal of Chemical & Engineering Data*, 70 (2025) 4880-4900. 10.1021/acs.jced.5c00578
F. Moradi, F. Bougie, A review of the application of deep eutectic solvents for metal recovery from diverse secondary sources, Journal of Molecular Liquids, 443 (2026) 128903. 10.1016/j.molliq.2025.128903.
B.B. Hansen, et. al. Deep Eutectic Solvents: A Review of Fundamentals and Applications, Chem. Rev. 2021, 121, 1232−1285. 10.1021/acs.chemrev.0c00385

1.5. Required initial knowledge and skills of the PhD candidate

Knowledge about general, physical, and polymer chemistry.
Ability to operate an atomic absorption spectrometer (AAS).
Self-discipline.
Motivation to achieve the goal (i.e. PhD degree).

1.6. Expected development of the PhD candidate's knowledge and skills

Ability to design deep eutectic solvents with desired properties.
Better understanding of physicochemistry of membrane transport.
The ability to work independently.
Gaining experience in analyzing according to principles of good laboratory practice (GLP).
The advanced ability of data processing and statistical/chemometric analysis.