Direct electrochemical reduction of selenium to achieve A-PRIME water treatment

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The project investigates the opportunity for direct electrochemical reduction of Se oxyanions to achieve the NAWI goal of A-PRIME (Autonomous, Precise, Resilient, Intensified, Modular, and Electrified) water treatment.

Project Background:

1. Aquatic selenium (Se) comes from mining, agricultural irrigation, hydraulic fracturing, and thermoelectric power generation.
2. Biological and physicochemical Se treatment show disadvantages, including large footprint, constant chemical dosing, and high cost.
3. Goal: To develop a direct electrochemical treatment technology that overcomes existing limitations.

Project Objectives:

Design: to determine appropriate materials that meet performance and cost targets

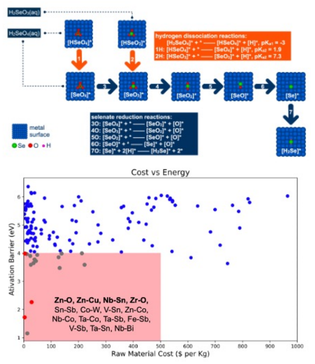
Synthesis: experimental synthesis and characterization for materials screening in Se reduction

Prototype: developing an electrochemical prototype system for reducing selenite and selenate from water

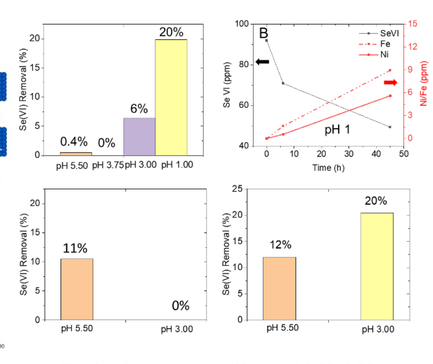
Assess: utilizing performance measurements and robustness tests, as well as techno-economic modeling for prototype device examination

Project Activities:

1. Screened over 1,500 bimetallic compounds and metal oxides to propose candidates of Zn-O, Zn-Cu, and Nb-Sn.
2. $Mg(OH)_2$, ZnO, and SnO_2 demonstrated effective Se(VI) removal at mild pH conditions (i.e., pH 5.5), which is crucial for practical water treatment applications.
3. Developed RuO_2 nanocatalysts grown on titanium plates $Ru_{0.9}Sn_{0.1}O_X$/TP electrode with high removal efficiencies of over 90% for Se(IV) concentrations of 0.1, 1, and 10 mM.
4. $Ru_{0.9}Sn_{0.1}O_X$/TP maintained similar performance even in the presence of competitive ions (Cl^-, SO_4^{2-}, and NO_3^-), underscoring its suitability for treating complex wastewater matrices.
5. Designed and optimized prototype Se(VI) electrocatalytic reactor using the selected catalyst to remove Se(VI) from complex water matrix and real FGD wastewater.
6. The average levelized cost of water for alternate selenium technologies was established from available literature.
7. Designed a TEA platform with data-driven process model to study the cost of electrochemical selenium removal.

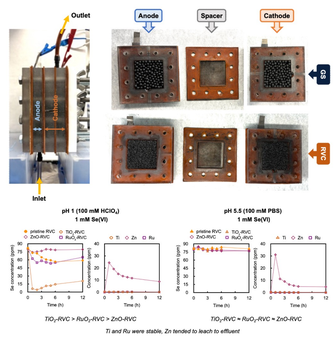


*top: Full Se(IV) and Se(VI) reaction diagram and **bottom**: the computational screening of Se(VI) electrode materials*

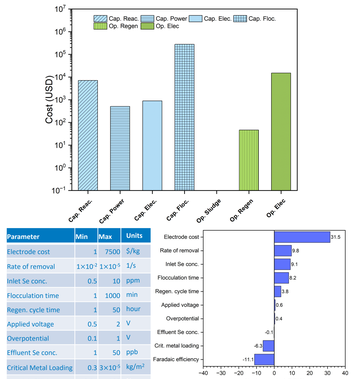


***a)** The Se(VI) removal by NiFe at pH 5.50, 3.75, 3.00, 1.00; **b)** Concentration change of Se(VI) and dissolved Fe/Ni from Ni-Fe alloy at pH 1 in two days; Se(VI) removal with **c)** SnO_2 and **d)** ZnO electrocatalyst at different pHs*

***top**: $Ru_{0.9}Sn_{0.1}O_x$ supported on Titanium plate SEM and TEM characterizations; **bottom**: In simulated wastewater containing 1 mM Se(IV) along with competitive anions (0.5 M Cl^-, 0.1 M SO_4^{2-}, 0.01 M NO_3^-)*



***top**: 3DER reactor with 3D carbon-based electrode fillers to reduce Se(VI) was investigated; **bottom**: Evaluation of various catalysts-coated RVC in continuous 3DER showed a better Se(VI) removal by TiO_2*



Parameter	Min	Max	Units
Electrode cost	1	7500	$/kg
Rate of removal	1×10^{-1}	1×10^{1}	1/s
Inlet Se conc.	0.5	10	ppm
Flocculation time	1	1000	min
Regen. cycle time	1	50	hour
Applied voltage	0.5	2	V
Overpotential	0.1	1	V
Effluent Se conc.	1	50	ppb
Critical Metal Loading	0.3	3×10^{3}	kg/m³
Faradaic Efficiency	0.01	100	%

***top:** Detailed cost breakdown of capital and operating costs from electrochemical reactor for base case. **bottom**: Parameter sensitivity analysis from WaterTAP model*

NAWI CONNECTIONS

Period of Performance: FY22Q2 – FY25Q2

Topic Area:

This project focuses on cutting-edge water treatment of selenium removal, for the purpose of providing a green, energy-efficient, and affordable water supply.

NAWI Leverage:

The research plan encompasses NAWI's "early-stage applied research philosophy," bringing together 5 PIs from 4 institutions with diverse backgrounds. Harnessing the tools developed via NAWI, the results and codes will also be shared via waterDAMS and waterTAP for future usage and reference.

KEY FINDINGS AND CONCLUSIONS

Key Findings:

1. $Mg(OH)_2$, ZnO, and SnO_2 demonstrated effective Se(VI) removal at mild pH conditions (i.e., pH 5.5), which is crucial for practical water treatment applications.
2. $Ru_{0.9}Sn_{0.1}O_X$/TP maintained similar performance even in the presence of competitive ions (Cl^-, SO_4^{2-}, and NO_3^-), underscoring its suitability for treating complex wastewater matrices.
3. The average LCOW of alternate selenium removal technologies with 15-year life span is 3.64 $/m³.
4. The LCOW of electrochemical selenium removal is 2.70 $/m³ for base case and it ranges from 2.64 – 3.53 $/m³ for parameter ranges tested.

Conclusion:

We have developed the 3DER and currently are working on applying the electrodes of various catalysts we discovered and testing using FGD wastewater.

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