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## Objective

Improve the understanding of uranium chemistry in molten salt reactors by studying U(III) and U(IV) in molten salt systems spectroelectrochemically.

## Introduction

### Advantages of Molten Salt Reactors (MSR)

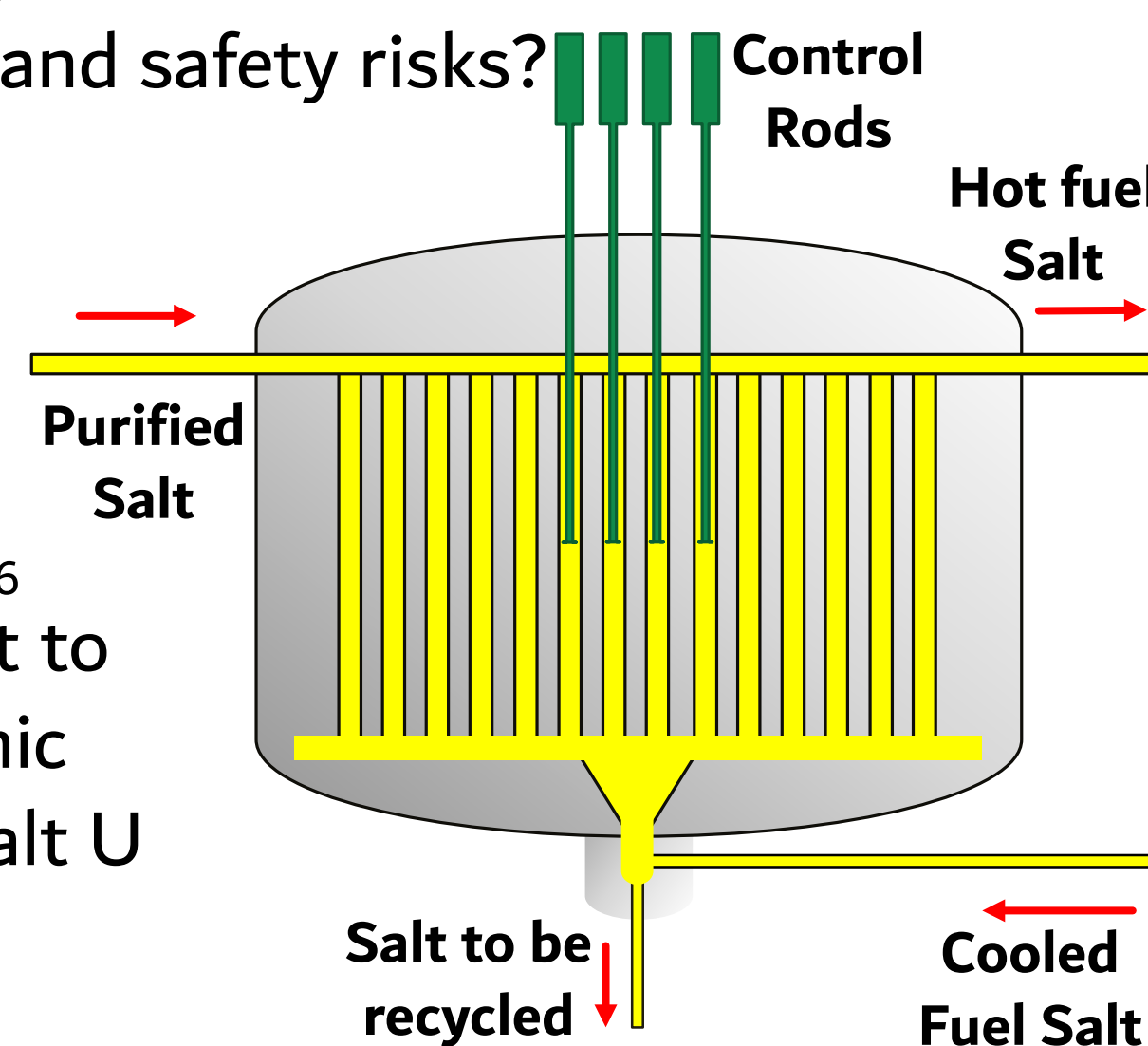
- Offer enhanced safety and efficiency through low pressure and high temperature operations
- Reduce the radiotoxicity of waste by 1/10,000<sup>th</sup> compared to conventional reactors
- Ease of enrichment and separation of fissile Pu

### Questions

- What chemistry is taking place that can contribute to **corrosion and precipitation effects**?
- How does the chemistry affect **proliferation concerns** and safety risks?

### Plan

- Measure the **diffusion coefficient** of U through molten salts
  - Test method:  $K_4Fe(CN)_6$
- Use diffusion coefficient to inform molecular dynamic simulations of molten salt U mixtures



## Methods

### Electrochemistry Experiments

- Materials**
  - Bob's cell as an electrochemical cell
  - Gamry 3000 Potentiostat to measure cyclic voltammograms (CV)
  - 5.007 mM  $K_4Fe(CN)_6$  in 100.15 mM  $KNO_3$
- Data Analysis**
  - Calculate the diffusion coefficient from a CV
    - Control potential
    - Measure resulting current for varying scan rates (50-500 mV/s)



$$i_p = 0.4463nFAC \left( \frac{nvFD}{RT} \right)^{1/2}$$

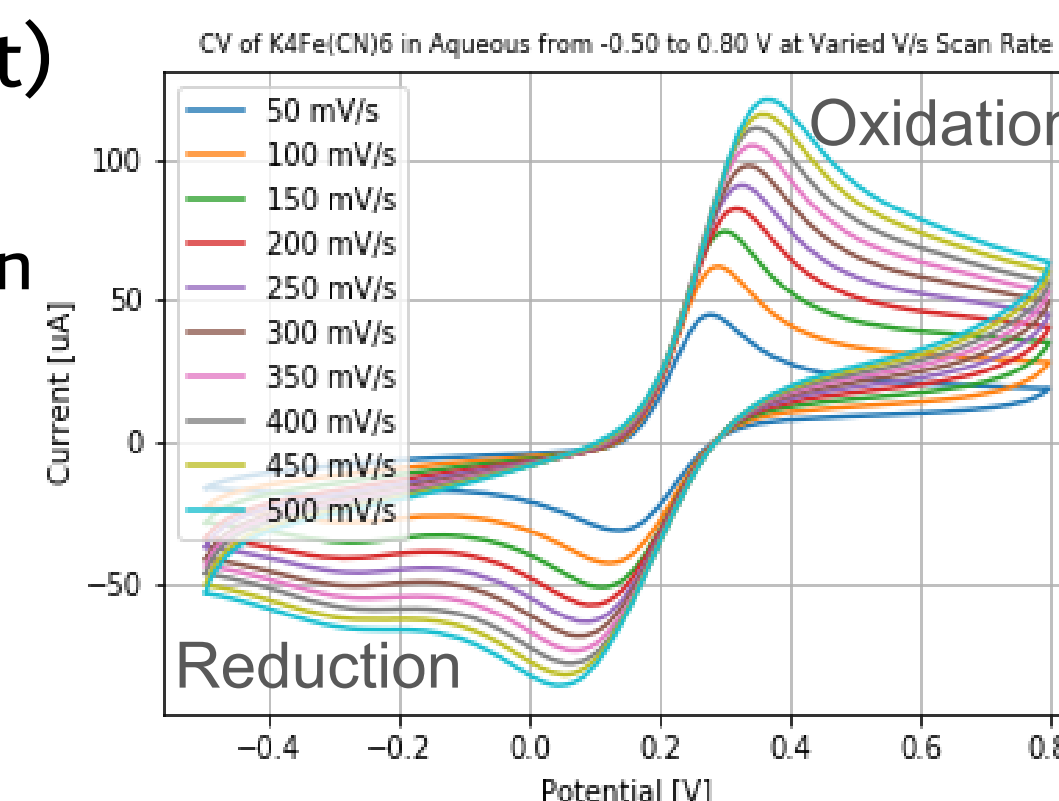
Randles-Sevcik Equation

## Results

### Cyclic Voltammogram (right)

#### Peak Drift

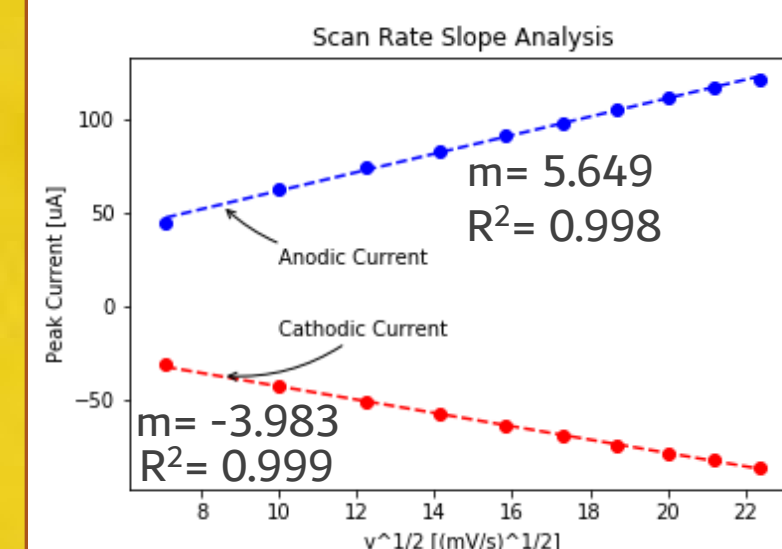
- A mild peak drift for oxidation and reduction with varying scan rate is seen in the CV
  - Oxidation peak drift was 0.0858 V
  - Reduction peak drift was 0.0929 V



### Diffusion Coefficient (D) (left)

#### Data from CV

- Use the slope and the R-S equation to calculate the diffusion coefficient
  - $D = 1.758 \cdot 10^{-6} \text{ cm}^2/\text{s}$
  - Currently investigating the 4 factor difference from known system



## Future Work

### Diffusion Coefficient

- Determine the diffusion coefficient for Eu(III) in LiCl-RbCl and 3 LiCl-2 CsCl eutectic melts
- Compare to literature
- Determine the diffusion coefficient for U(III) and U(IV) in molten salt mixtures
- Use results to inform molecular dynamics

### Extended X-ray Absorption Fine Structure (EXAFS)

- Determine the local coordination environment of U in a chloride eutectic molten salt
- Determine bond distance between bonded salt constituents relative to uranium

### Raman Spectroscopy

- Define the bonding characteristics of U with the salt constituents

Diffusion Coefficient

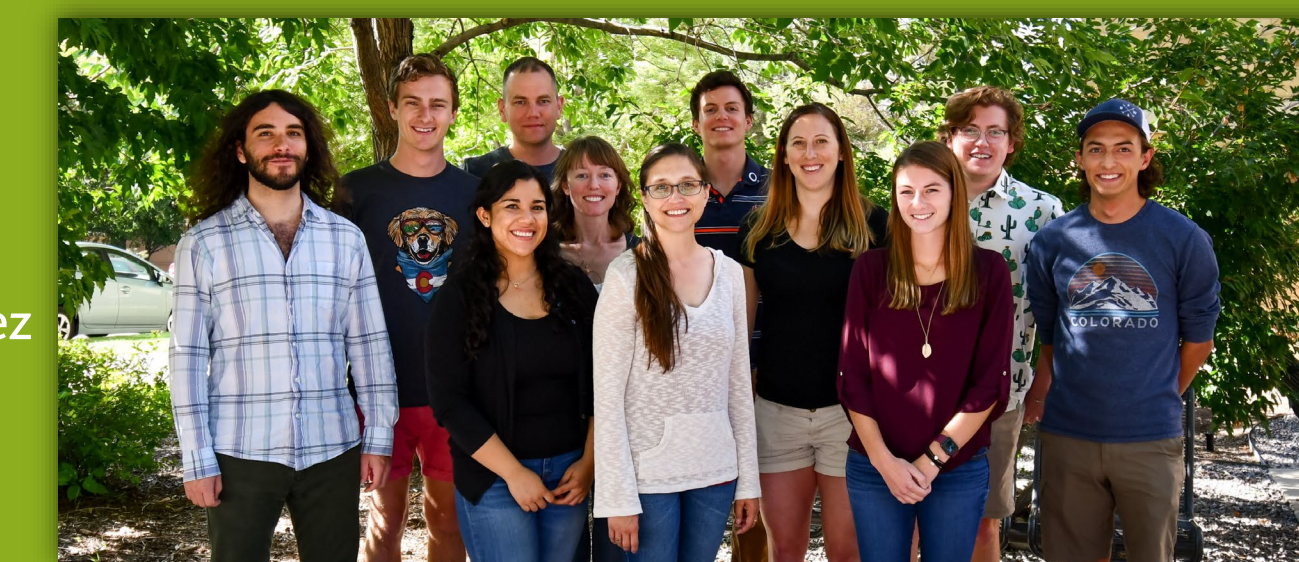
EXAFS

Raman

## Shafer Group

Front: Andrew Fletcher, Vanessa Linero, Erin Bertelsen, Jennifer Shafer, Me, Jacob Tellez

Back: Eric Norfleet, Kevin Pastoor, Jessica Jackson, Brian Arko, Ian Wilkinson



## References

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## Acknowledgements

Funding for this research was provided by the NNSA and the consortium for Enabling Technologies and Innovation. Additional thanks to Georgia Tech for the invitation and opportunity to present my research.