Characterization and Modeling of an All-Aqueous Thermally Regenerative Redox Flow Battery

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Project Title: Development of an All-Aqueous Thermally Regenerative Redox Flow Battery to Support Fossil Fuel Assets

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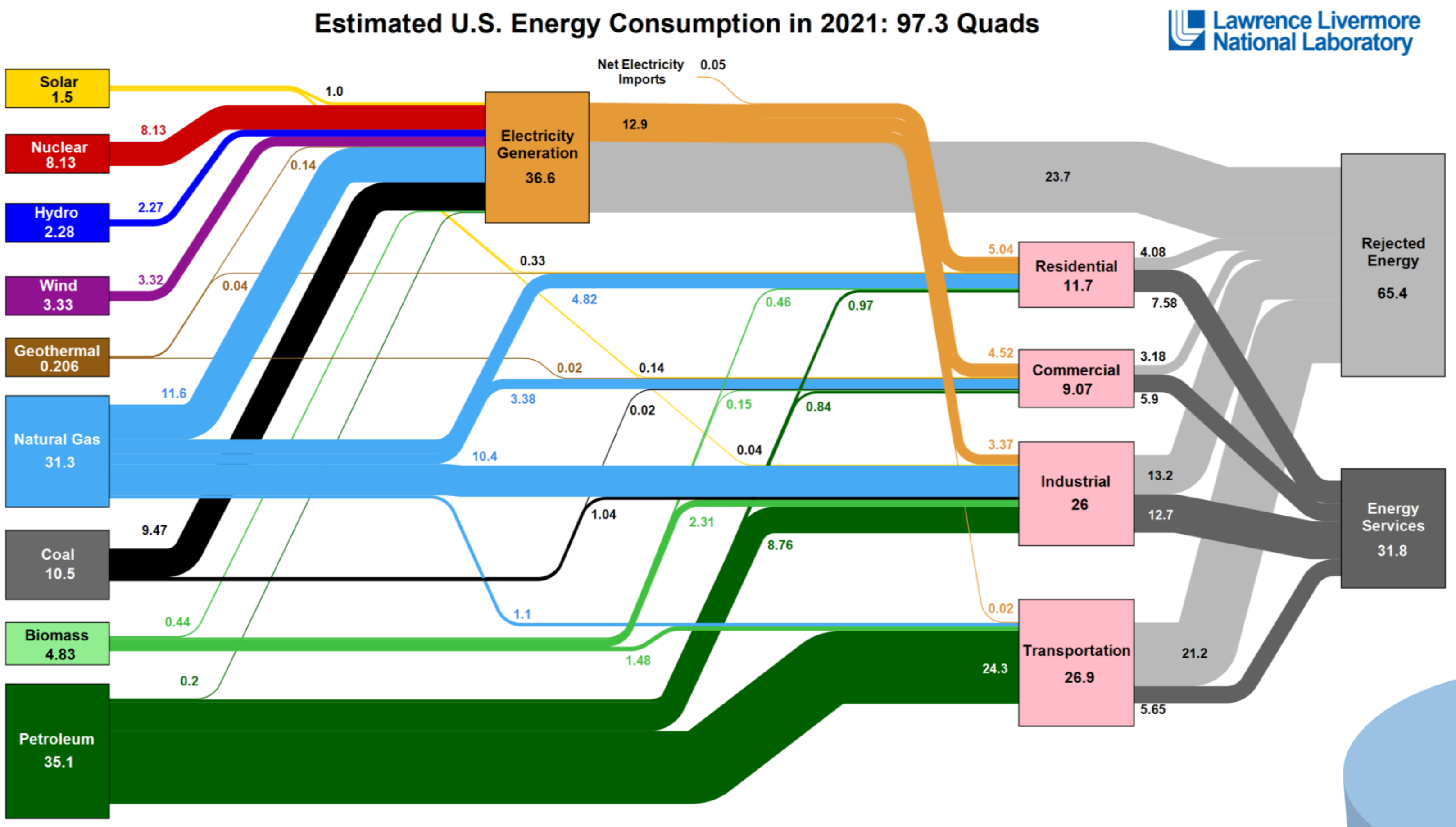
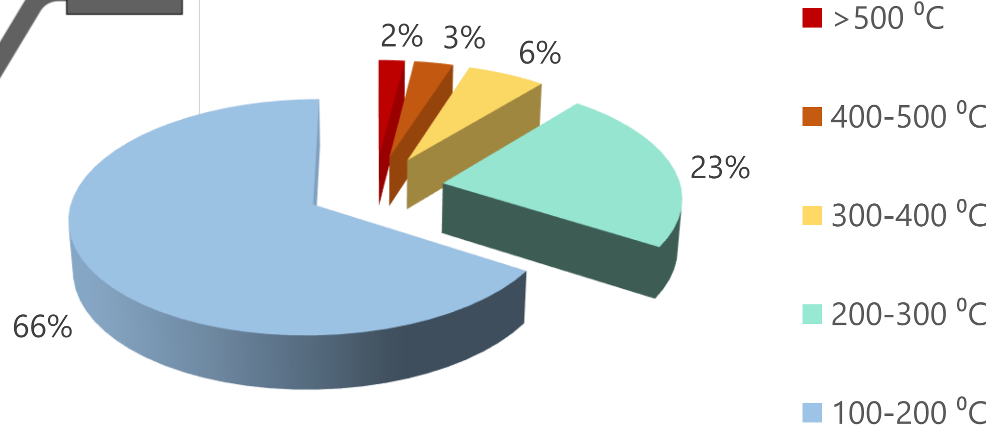
College of Engineering

U.S. DEPARTMENT OF ENERGY | NATIONAL ENERGY TECHNOLOGY LABORATORY

Award Number: FE0032030-FOA 2332

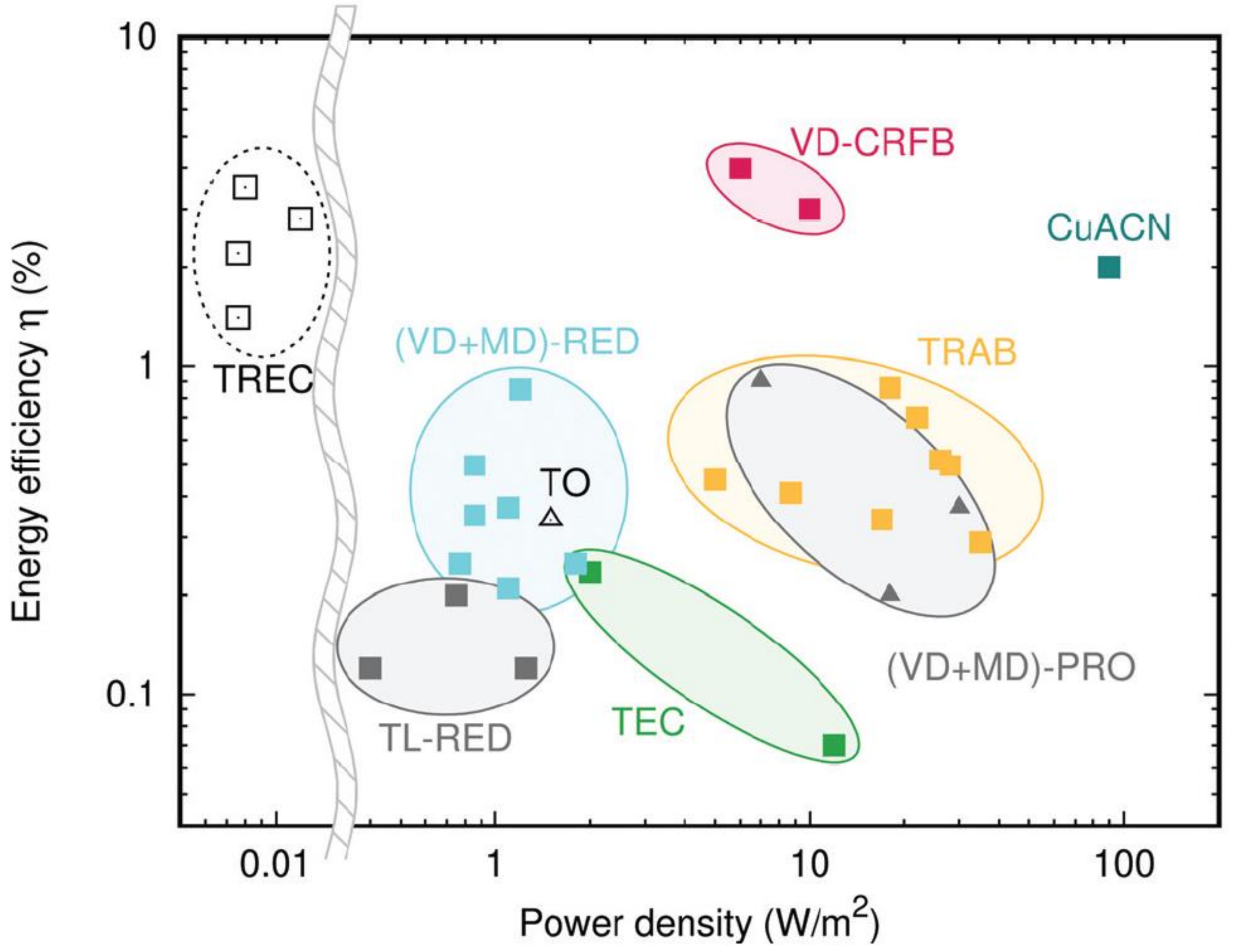
"Low-grade" heat is abundant





https://flowcharts.llnl.gov/sites/flowcharts/files/2022-04/Energy_2021_United-States_0.png
Adapted from "Some efficient solutions to recover low and medium waste heat: competitiveness of the thermoacoustic technology", Haddad et al., 2014

Many technologies can take advantage of low-grade heat



"Innovative technologies for energy production from low temperature heat sources: critical literature review and thermodynamic analysis", Brogioli and La Mantia, 2021

Flow battery + distillation column = Thermally regenerative battery

Flow battery:

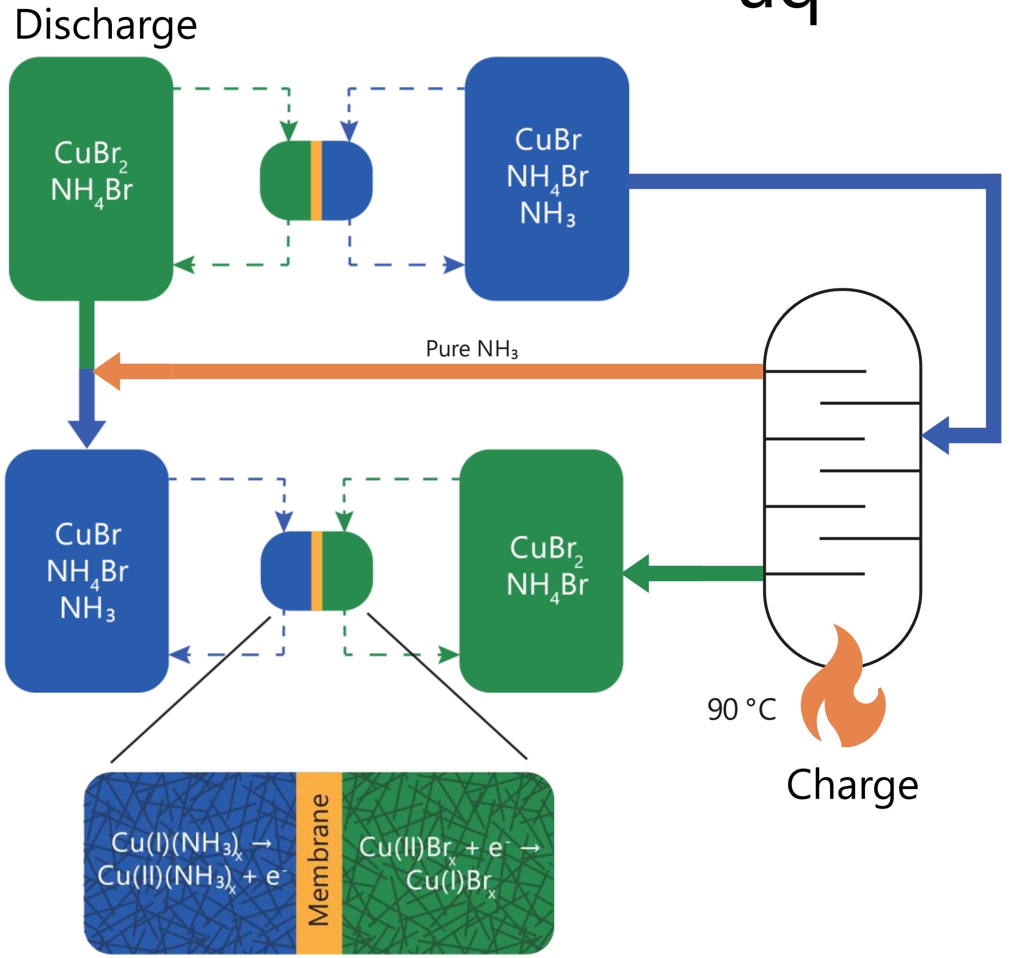
Large scale batteries

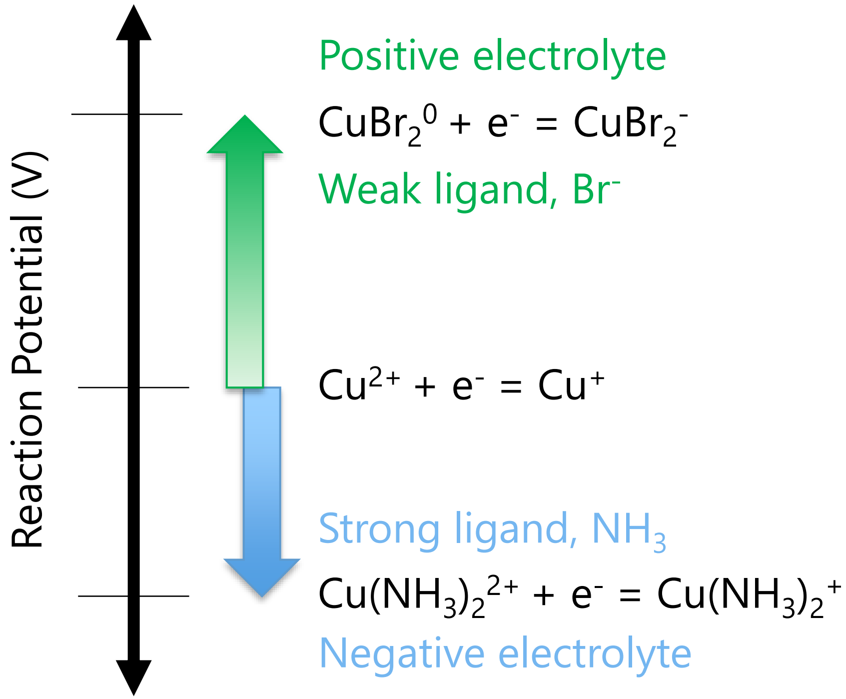
Distillation column:

Large scale thermal separations

https://organics.co.uk/en/products/20/ammonia-stripping-systems
https://www.cellcube.com/casestudy/gw-microgrid-campus/

How the All-Aqueous Cu-TRAB (Cu_{aq}-TRAB) works





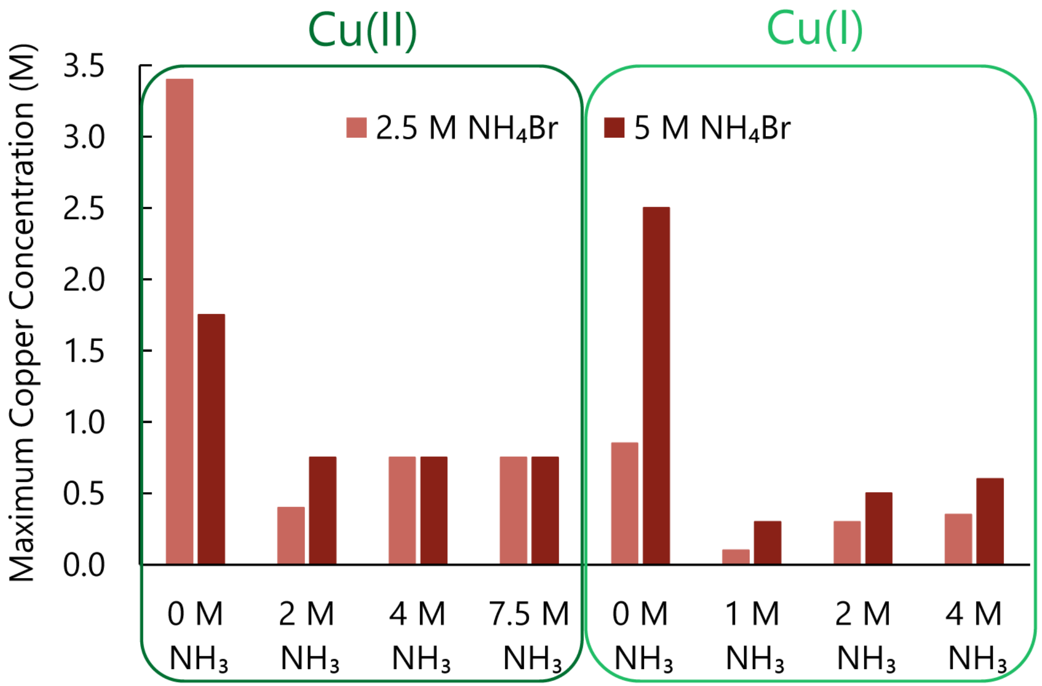
"Power and energy capacity tradeoffs in an all-aqueous copper thermally regenerative ammonia battery", Cross, et al., 2022

Milestone 1: Quantify thermodynamic energy storage density

Milestone 2: Preliminary power density assessment using a COMSOL model

Solubility limits and equilibrium potentials were measured at varying ligand concentrations

Ligand	Concentration (mol kg^{-1})	Potential (mV)
Br^-	4	648 ± 2
	1	518 ± 1
Cu(I,II)	"Standard"	150
NH_3	1	23 ± 5
	4	-47 ± 1



- Cell potential can reach ~700 mV with high concentration
- Cu(I)NH_3 complex limits solubility to 0.6 M

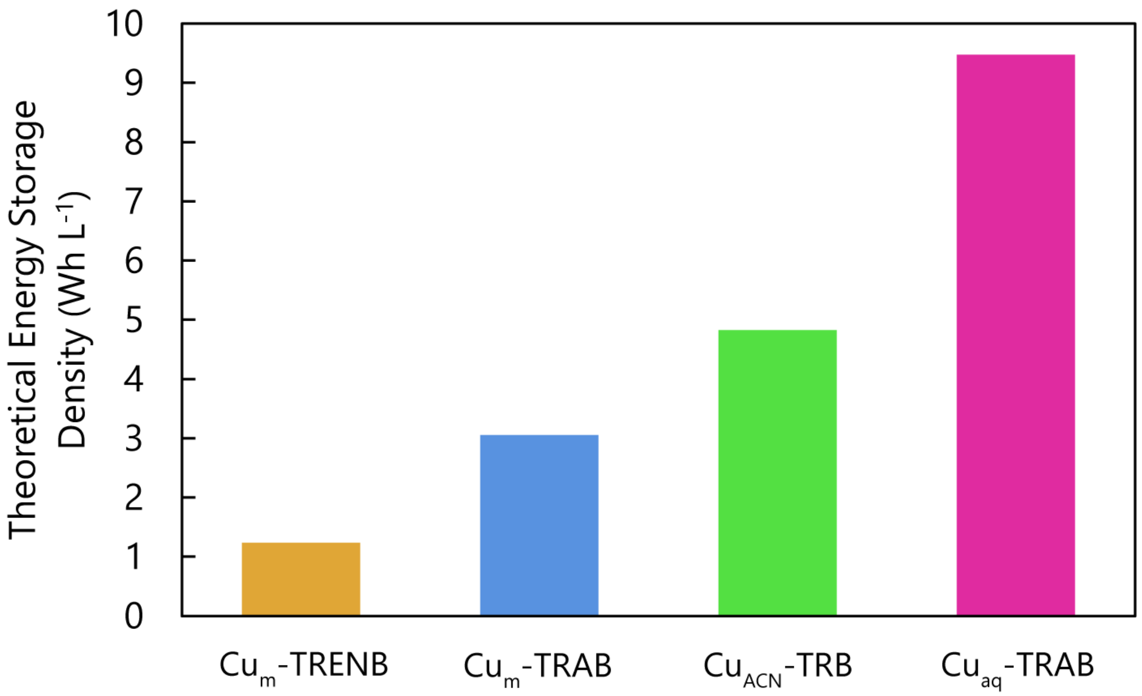
"An All-Aqueous Thermally Regenerative Ammonia Battery Chemistry Using Cu(I,II) Redox Reactions", Springer, et al., 2021
"Power and energy capacity tradeoffs in an all-aqueous copper thermally regenerative ammonia battery", Cross, et al., 2022

Theoretical energy density was estimated to be double previous TRB chemistries

Cell potential: ~700 mV

Max solubility: 0.6 M

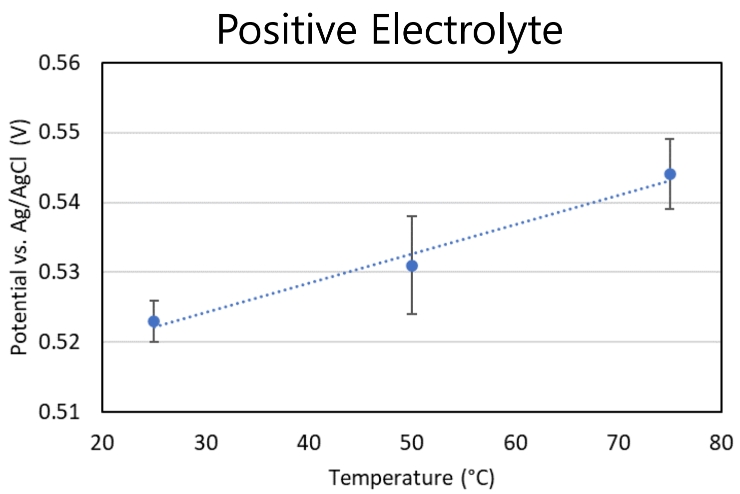
$$Max\ energy\ density = E^0_{cell} * c_{max} * F$$

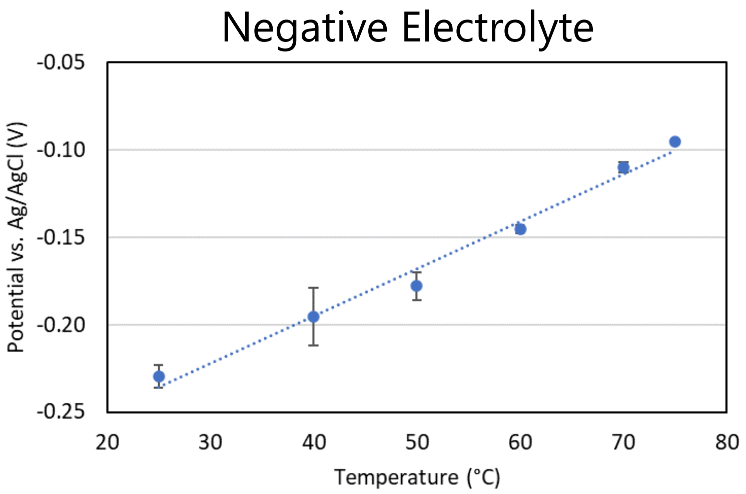


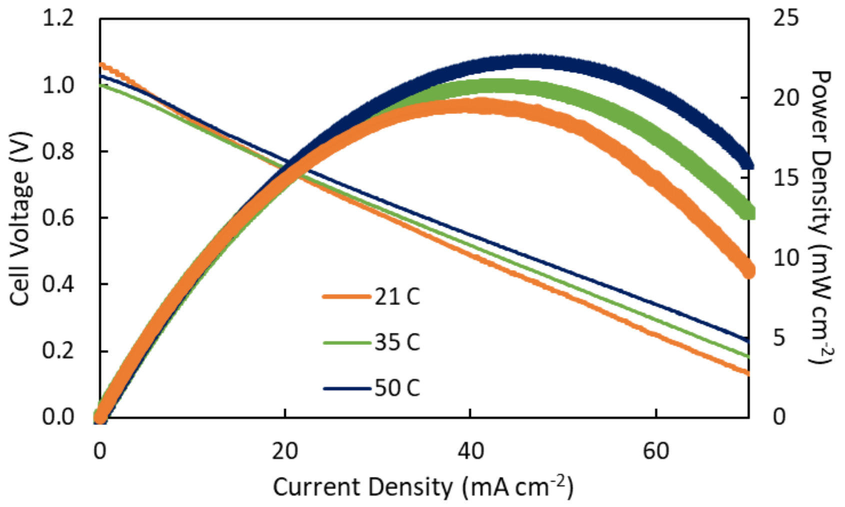
Milestone 1: Quantify thermodynamic energy storage density

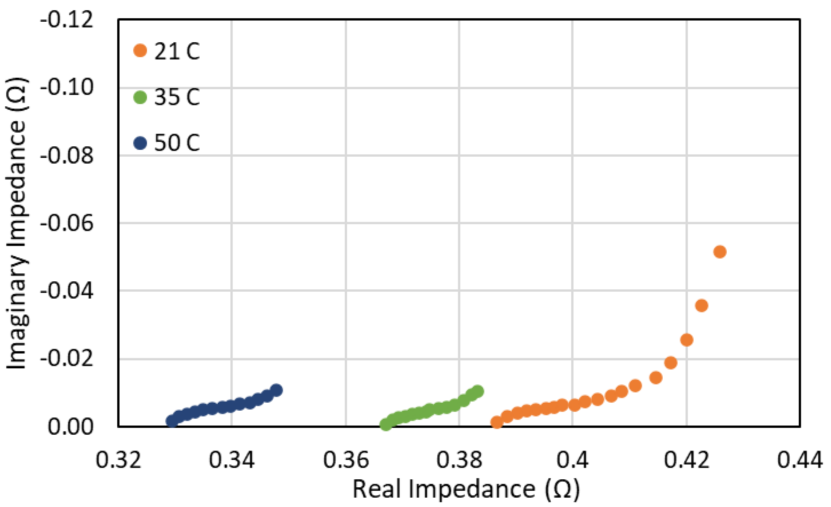
"Power and energy capacity tradeoffs in an all-aqueous copper thermally regenerative ammonia battery", Cross, et al., 2022

Power density can be improved at elevated temperatures through lower ohmic losses



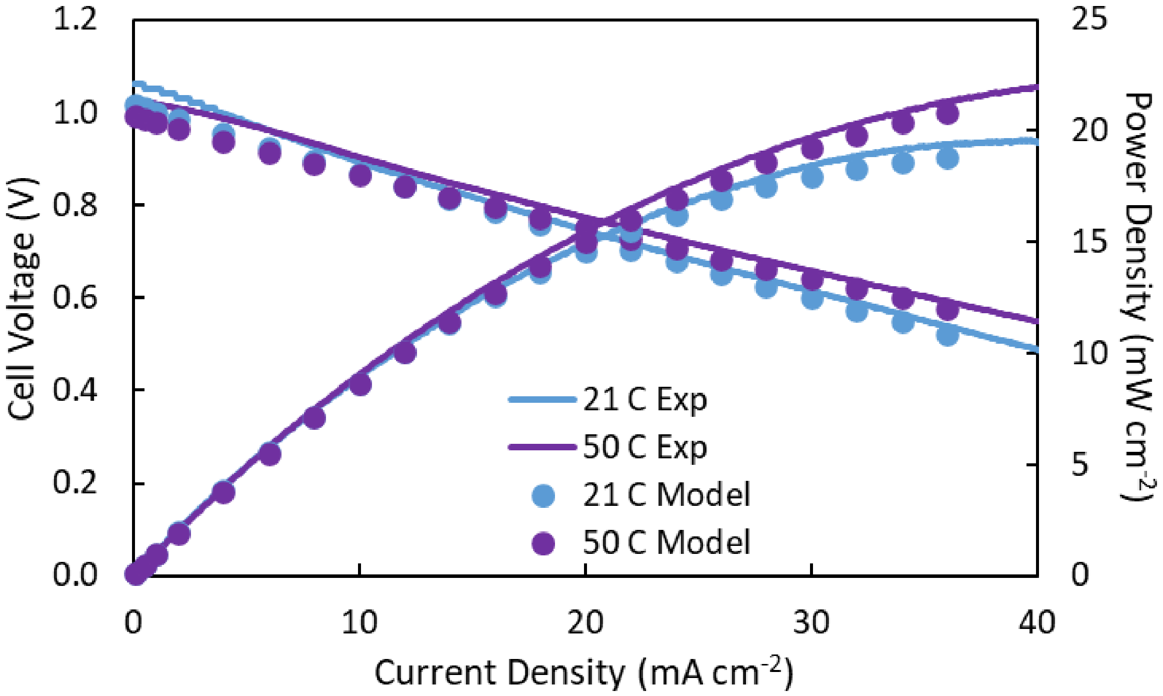


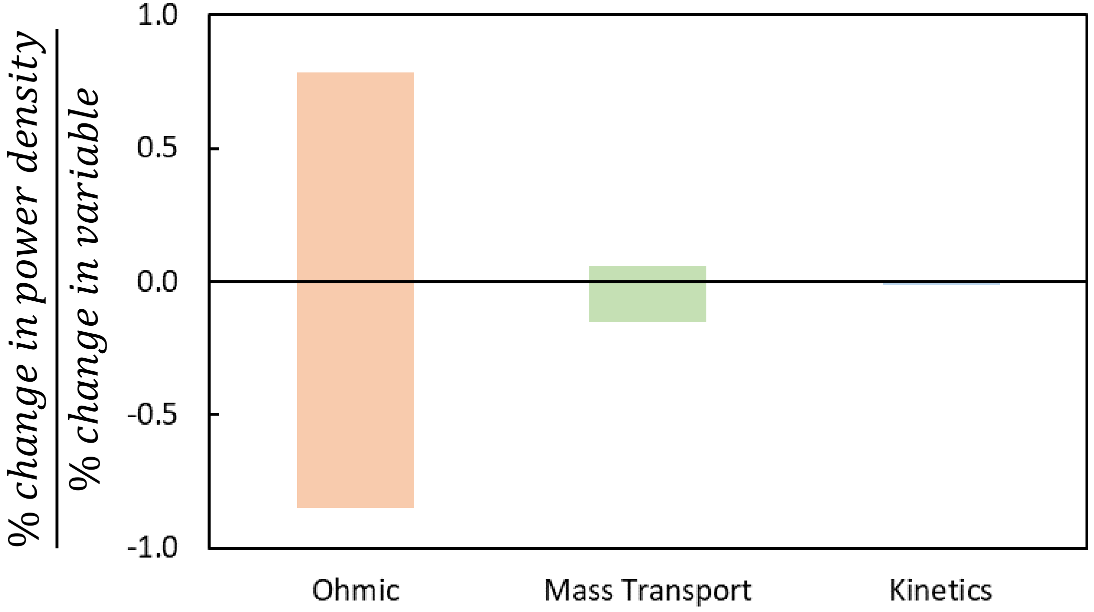




Unpublished data

Power density is simulated accurately with our model and shows the importance of ohmic losses





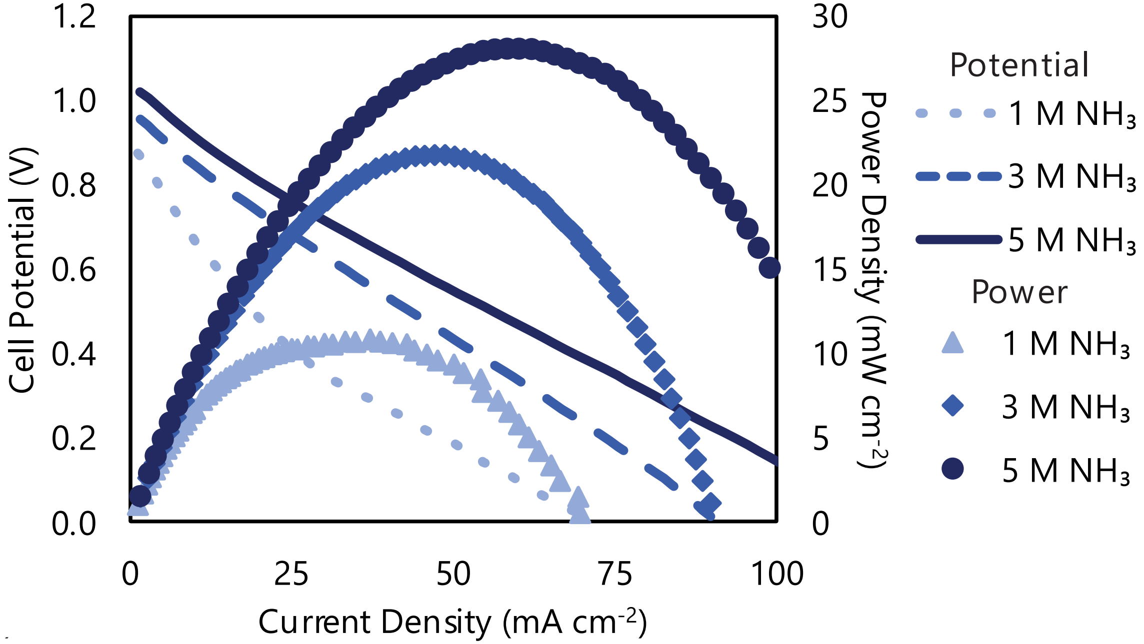
0.5 M $CuBr_x$, 5 M NH_4Br, 4 M NH_3
99.5% SOC, Nafion 117, 50 ml min^{-1}

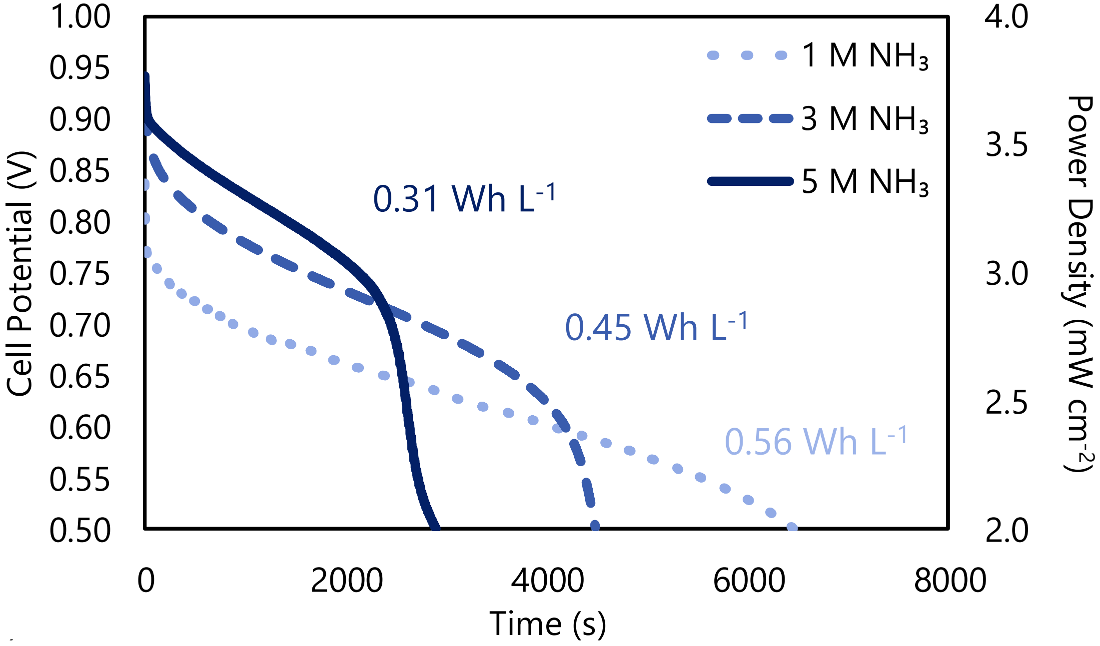
Milestone 2: Preliminary power density assessment using a COMSOL model

Unpublished data

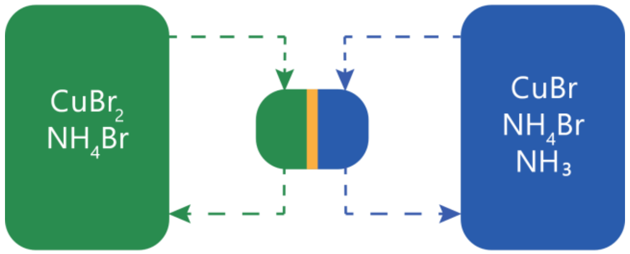
How do the electrolyte composition and operating parameters impact power and energy output?

Increasing ammonia concentration increases power density





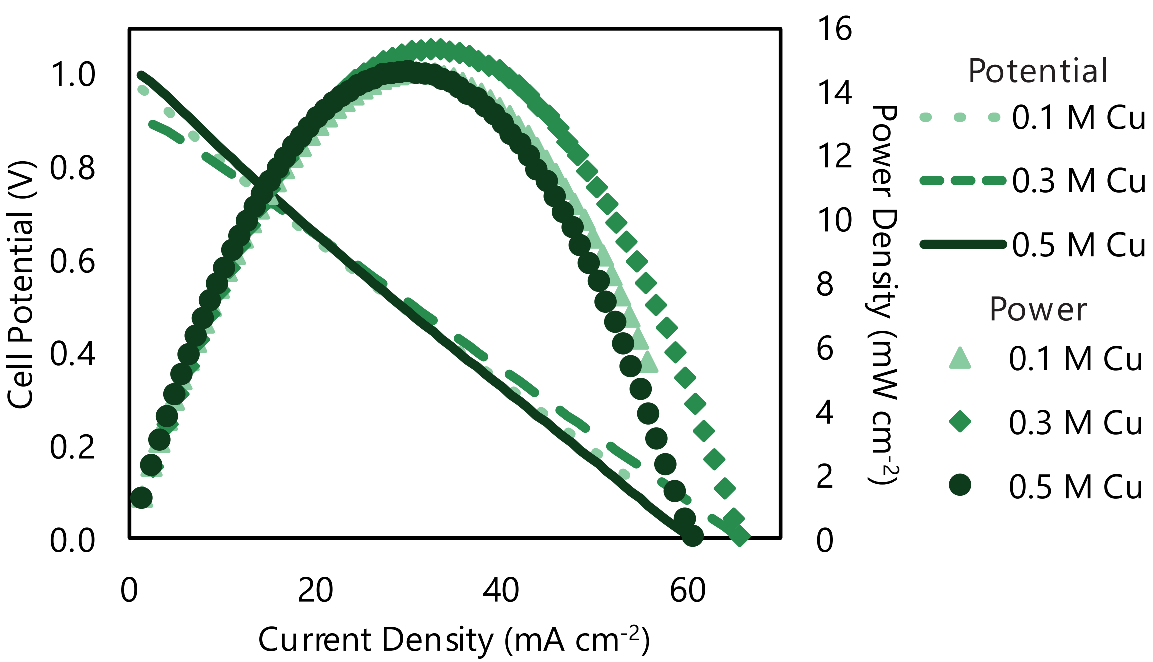
0.1 M Cu, 5 M NH_4Br
200 ml min^{-1}, 99% SOC
Nafion 117

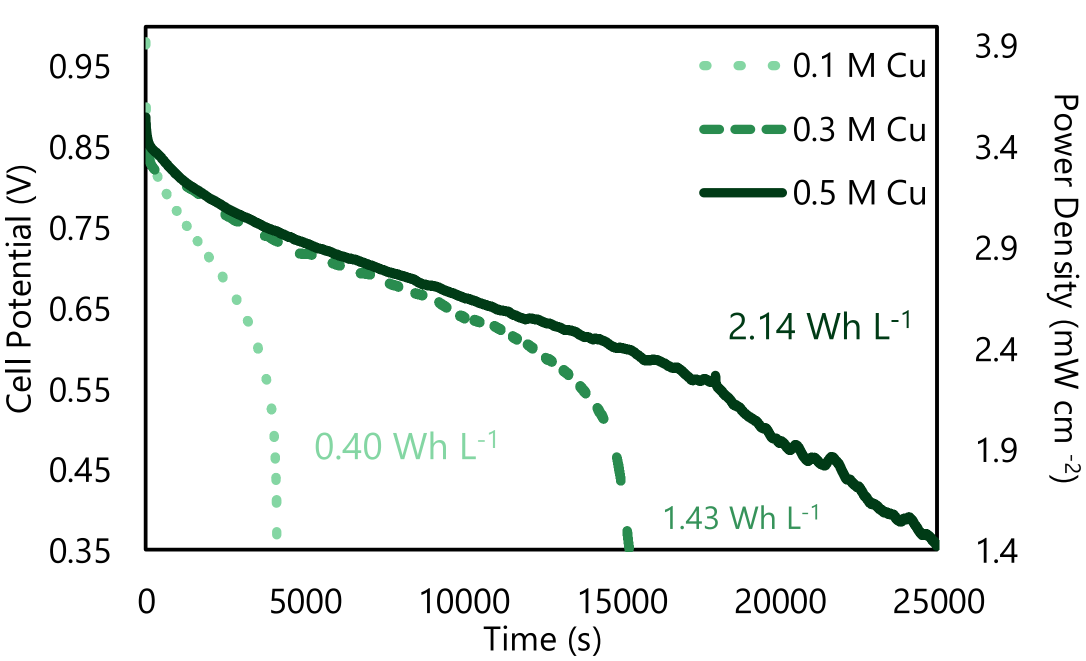


4 mA cm^{-2} applied current
99% SOC initial

"Power and energy capacity tradeoffs in an all-aqueous copper thermally regenerative ammonia battery", Cross, et al., 2022

Higher copper concentration does not change power and increases energy density



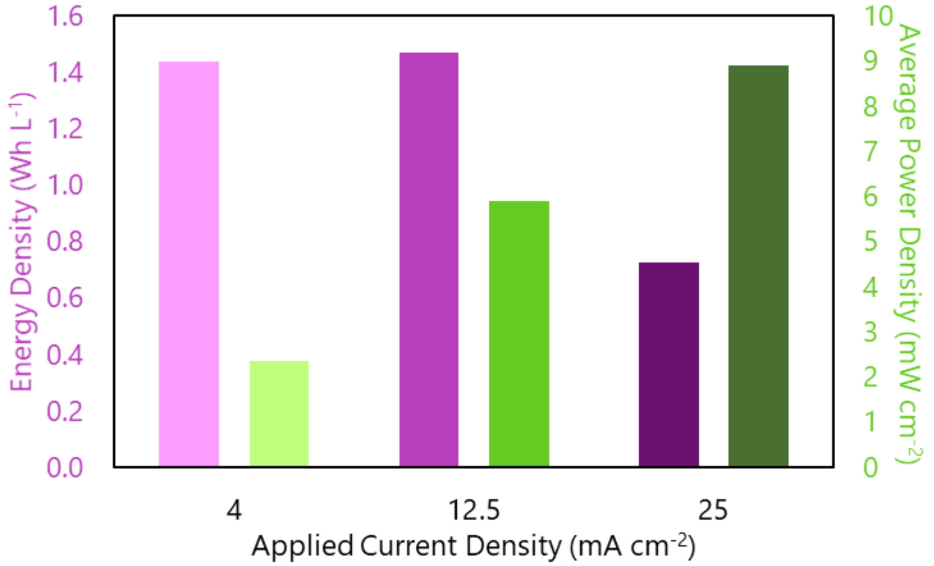


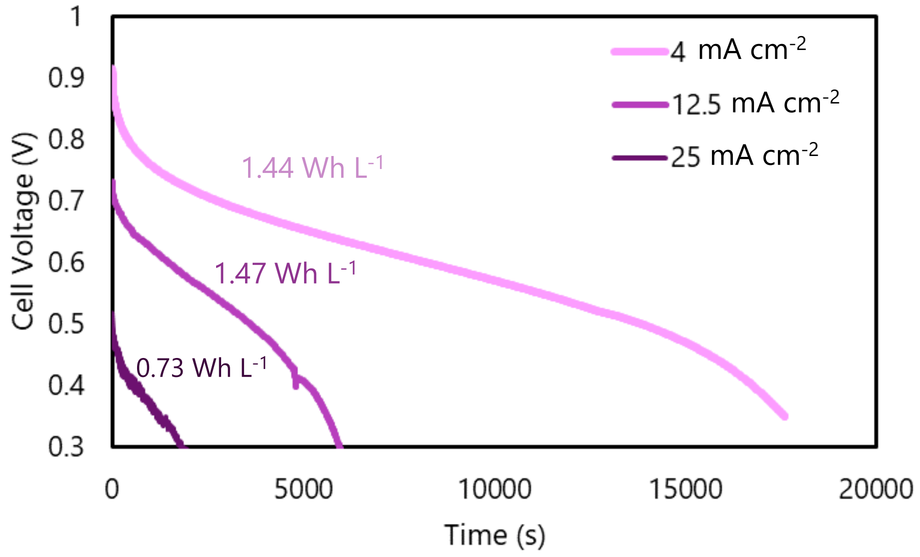
5 M NH_4Br, 4 M NH_3
50 ml min^{-1}, 99% SOC
Nafion 117

4 mA cm^{-2} applied current
99% SOC initial

"Power and energy capacity tradeoffs in an all-aqueous copper thermally regenerative ammonia battery", Cross, et al., 2022

Increasing applied current can counteract ammonia crossover



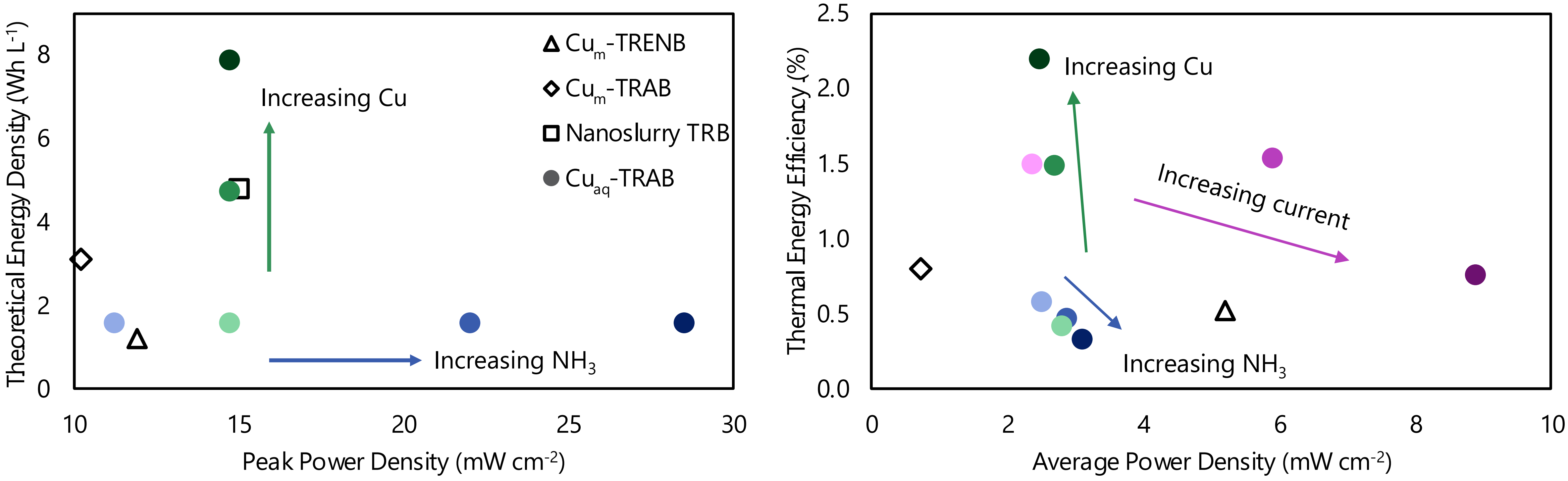


- Evidence of a tradeoff between overpotential and discharge time
- Higher applied currents lead to higher overpotentials and less usable energy
- Higher applied currents decrease discharge time which provides less time for parasitic crossover

0.3 M Cu, 5 M NH_4Br, 1 M NH_3
200 ml min^{-1}, 99% SOC
Nafion 117

"Power and energy capacity tradeoffs in an all-aqueous copper thermally regenerative ammonia battery", Cross, et al., 2022

The Cu_{aq}-TRAB performs well compared to previous TRAB chemistries



- Large increases in peak power and theoretical energy density

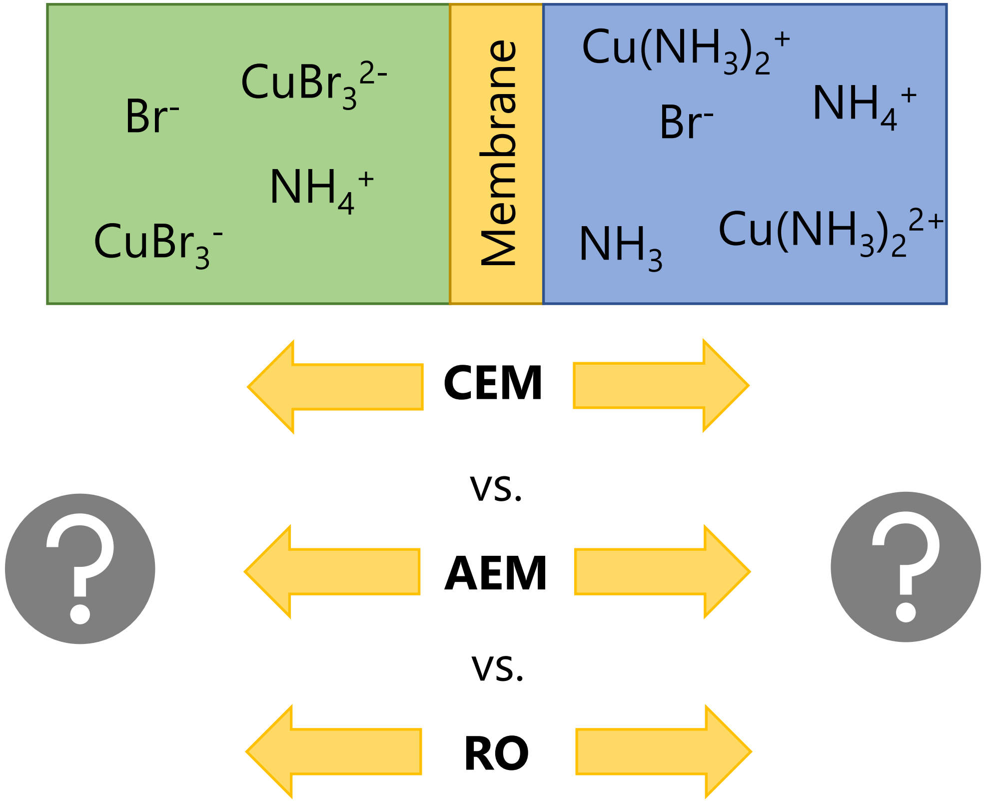
"Power and energy capacity tradeoffs in an all-aqueous copper thermally regenerative ammonia battery", Cross, et al., 2022

Milestone 1: Quantify thermodynamic energy storage density

Milestone 2: Preliminary power density assessment using a COMSOL model

Milestone 3: Identify performance characteristics of suitable membrane types

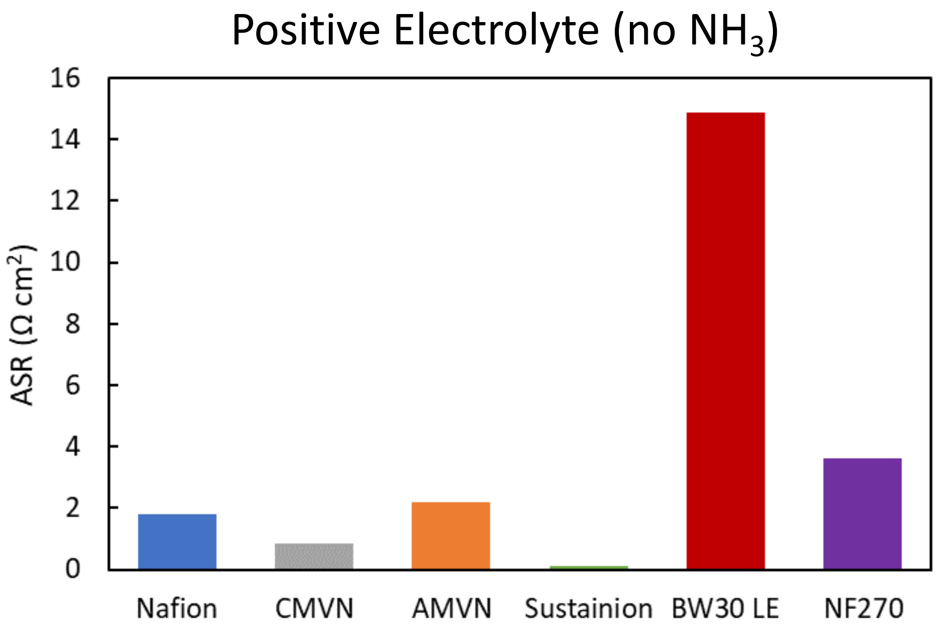
Membranes are being evaluated for peak and long-term performance

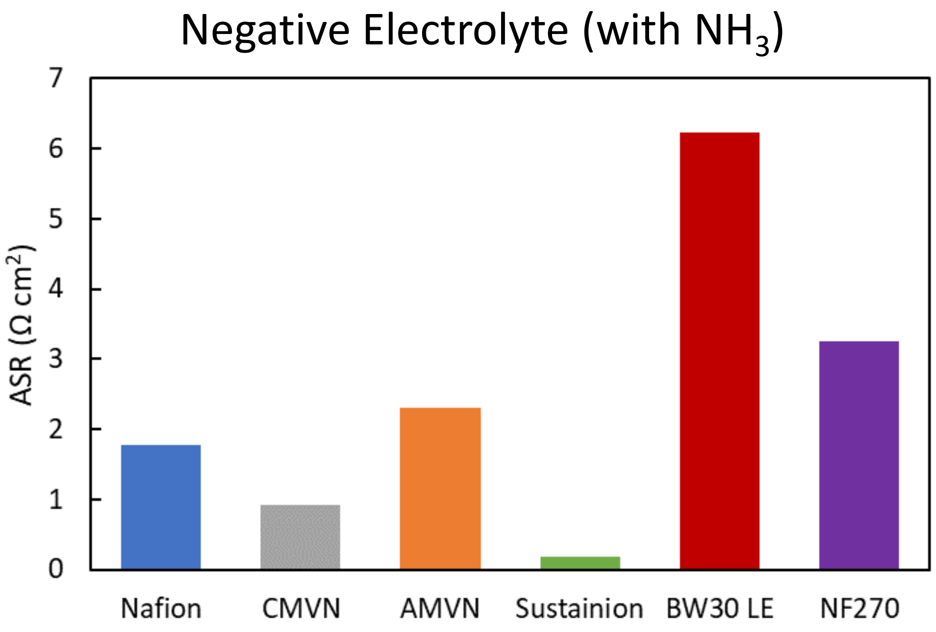


Resistivity

Permeability

Resistance data indicates that membranes can increase battery performance





- Charged membranes had lowest resistances
- NF membrane had low resistance, but will likely have high permeability
- Thin Sustainion membrane had best performance

Unpublished data

Journal of The Electrochemical Society, 2021 **168** 070523

Links to our papers:

An All-Aqueous Thermally Regenerative Ammonia Battery Chemistry Using Cu(I, II) Redox Reactions

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Power and energy capacity tradeoffs in an all-aqueous copper thermally regenerative ammonia battery

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Thank you and please contact us if you have any questions!

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