Oak Ridge National Laboratory

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OE Storage, FY26 : Understanding the Impact of Hydrogen evolution and crossover on Performance of Vanadium Redox Flow Battery

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U.S. DEPARTMENT of ENERGY

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Project Overview

Project Goal: Develop a high-fidelity physics-based framework for degradation simulation of Vanadium Redox Flow Battery (VRFB).

i. VRFB are prime candidates for long-duration large-scale energy storage with limited deployment already in the field.

ii. Design the computational architecture to handle both the complex electrical circuit and fluid dynamics.

Current Practices: Typical system scale models for VRFB use (a) simplified equivalent circuit models, (b) lack accurate coupling of the electrochemical, electrical, and fluid flow components. (c) Critical degradation modes, such as hydrogen evolution reaction (HER), and system inefficiencies, like flow maldistribution, have not been considered in any meaningful way on a VRFB stack.

Why ORNL: We are well positioned with the HPC facilities for efficient design and performance analysis of VRFB. While also aiding in generating significant long-term cycling synthetic data for AI/ML efforts. Strong synergies with the GRID-C team on integrating the physics model with the Controller Hardware-in-the-loop (CHIL) platform.

Innovation: Our current approach is (a) computationally efficient for design, and analysis of VRFB that can simulate a stack, (b) utilizes fully physics-based model that can resolve the various phenomena critical to VRFB (c) with resolved crucial degradation mechanisms and system inefficiencies, and (d) able to make long-duration life-cycle predictions of the battery.

Impact: Cycles till significant loss of usable battery capacity evaluated under diverse configurations. Strategy to enhance performance formulated — exploit the newly discovered capacity retention due to competition between crossover and HER degradation. Shaping of long-term discharge capacity due to flow maldistribution unearthed. Enables aging-informed design and control strategies for more durable, reliable, and cost-effective grid-scale flow battery deployment.

Alignment: This aligns well with the DOE-OE mission, through aiding the development of cost-effective grid scale energy storage to improve safe and reliable power delivery

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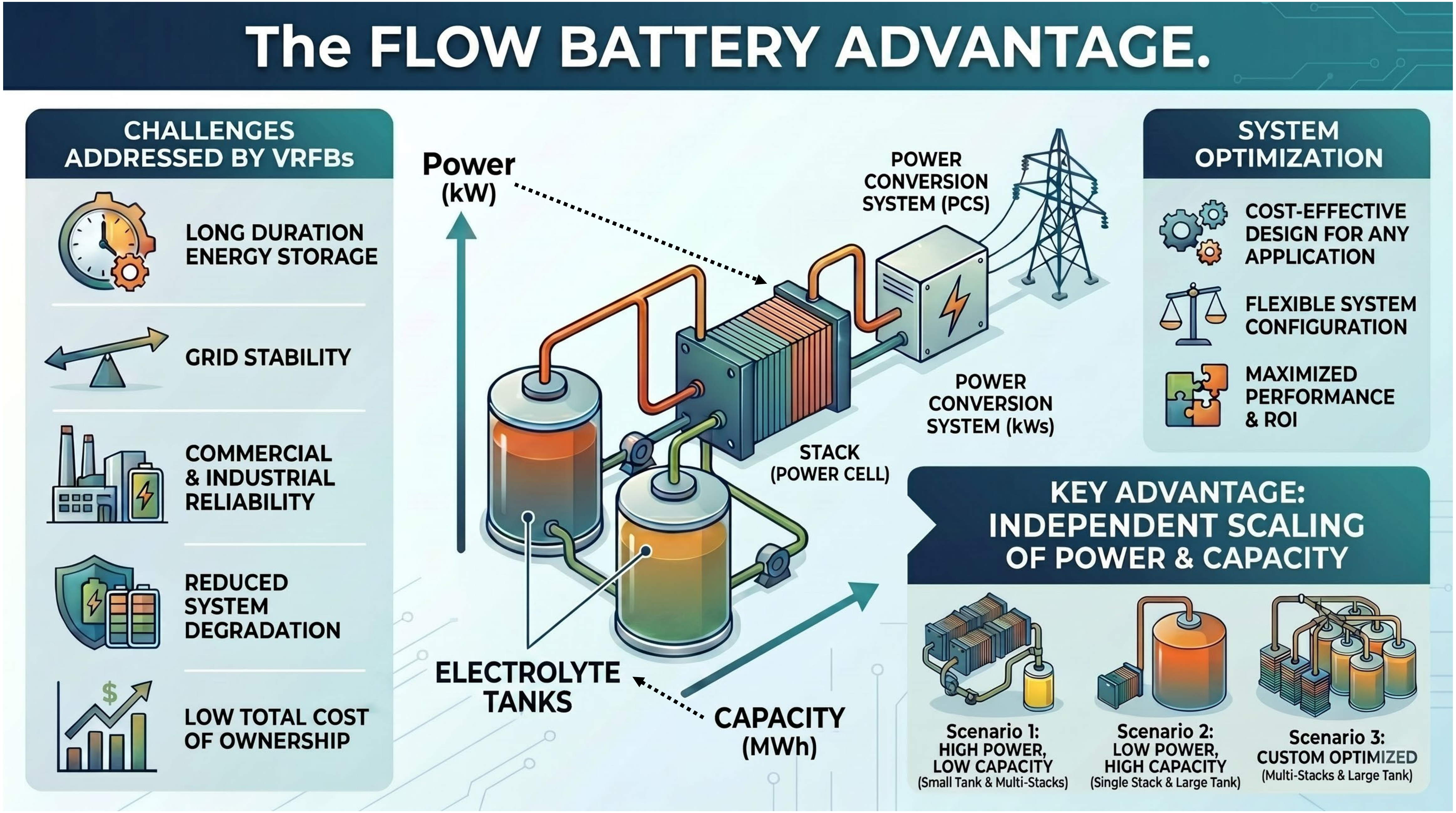
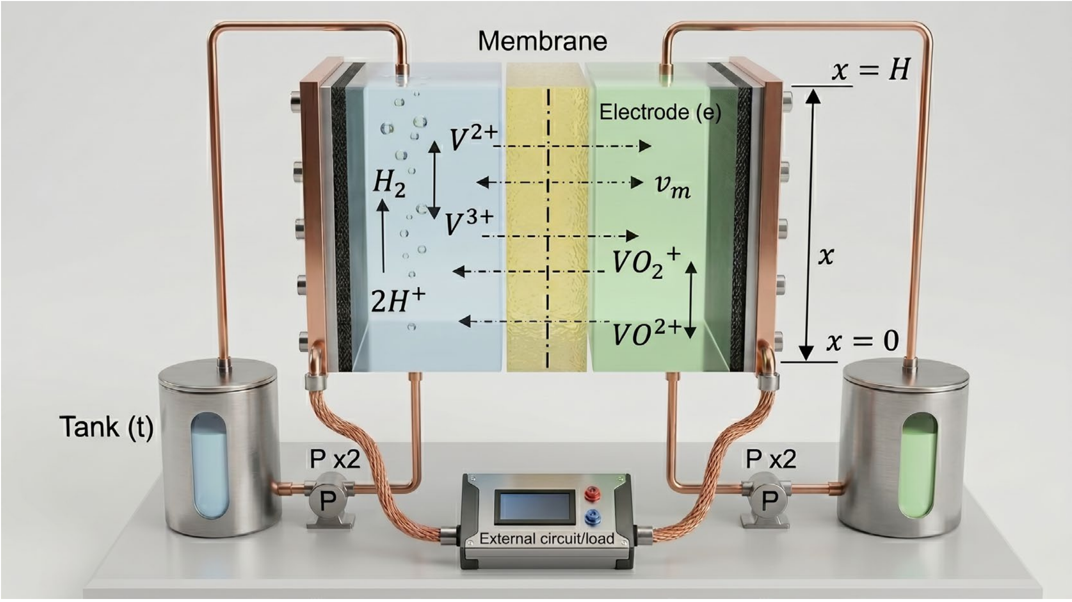
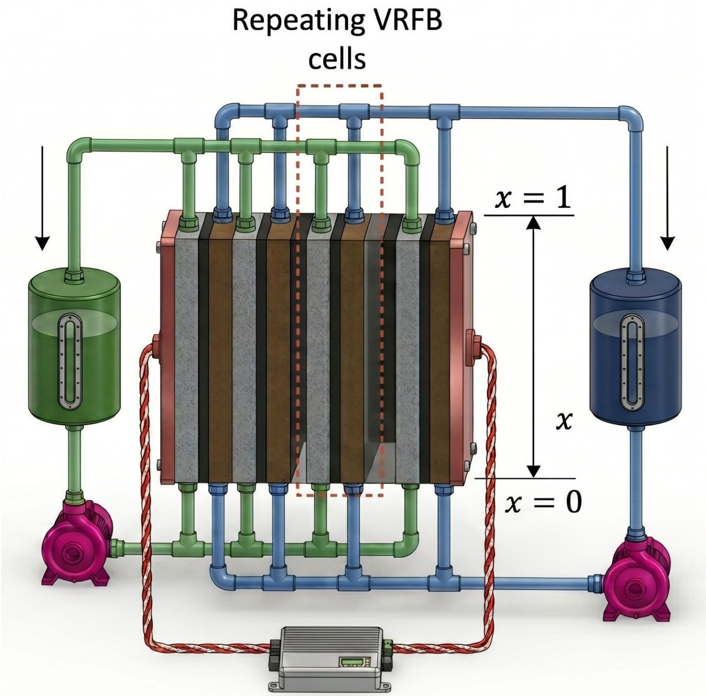

The FLOW BATTERY ADVANTAGE.
CHALLENGES ADDRESSED BY VRFBs
LONG DURATION ENERGY STORAGE
GRID STABILITY
COMMERCIAL & INDUSTRIAL RELIABILITY
REDUCED SYSTEM DEGRADATION
LOW TOTAL COST OF OWNERSHIP
Power (kW)
POWER CONVERSION SYSTEM (PCS)
POWER CONVERSION SYSTEM (kWs)
STACK (POWER CELL)
ELECTROLYTE TANKS
CAPACITY (MWh)
SYSTEM OPTIMIZATION
COST-EFFECTIVE DESIGN FOR ANY APPLICATION
FLEXIBLE SYSTEM CONFIGURATION
MAXIMIZED PERFORMANCE & ROI
KEY ADVANTAGE: INDEPENDENT SCALING OF POWER & CAPACITY
Scenario 1: HIGH POWER, LOW CAPACITY (Small Tank & Multi-Stacks)
Scenario 2: LOW POWER, HIGH CAPACITY (Single Stack & Large Tank)
Scenario 3: CUSTOM OPTIMIZED (Multi-Stacks & Large Tank)

Vanadium Flow battery Framework for Life-cycle Emulation



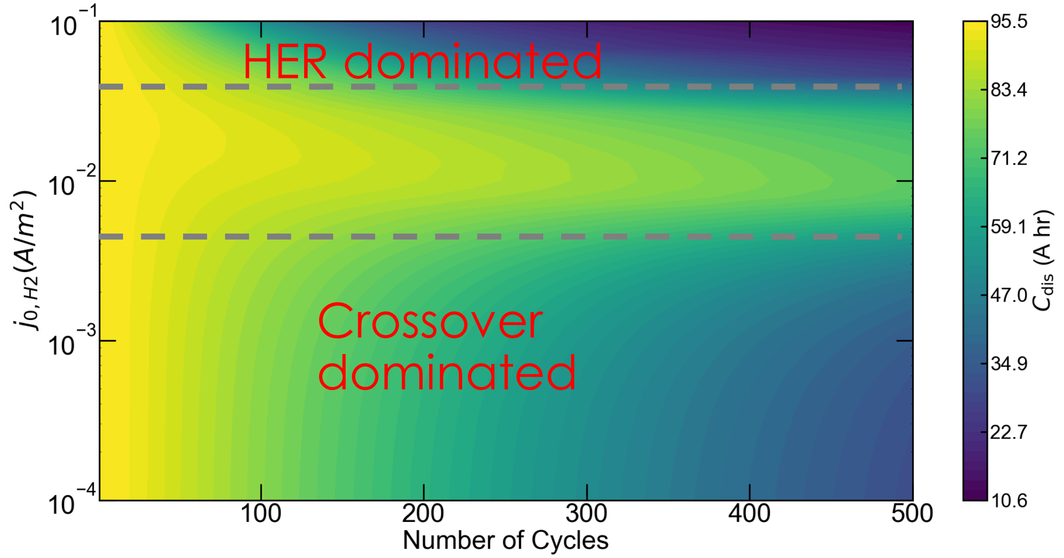


- High fidelity pseudo 2-D experimentally validated model of VRFB cell.
- Electrochemical reaction, mass transport, and fluid dynamics resolved.
- Degradation: Ion and electrolyte crossover, self-discharge reaction, Hydrogen Evolution Reaction (HER).

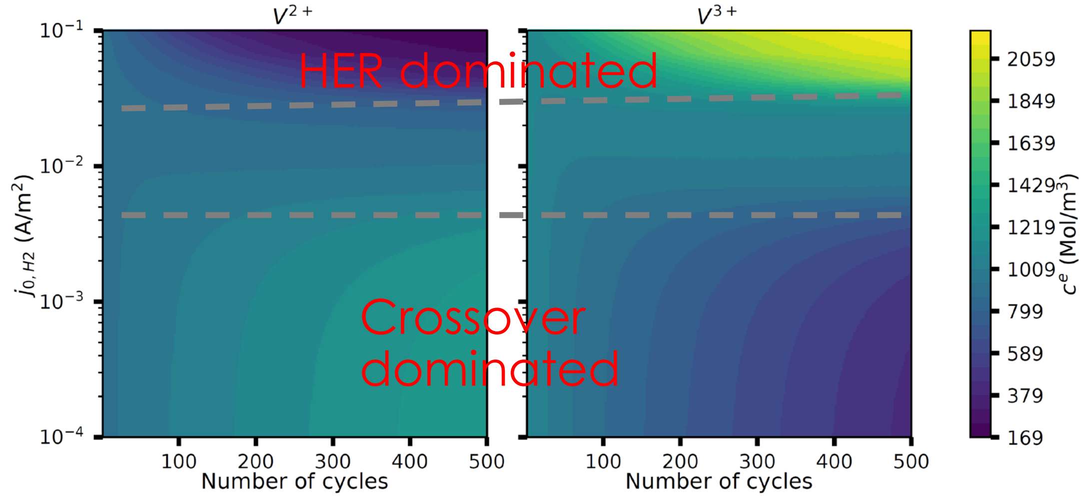
- Stack performance investigated by arranging cells electrically in series but parallel for electrolyte flow.
- Flow maldistribution modelled via throttling flow to one cell in the stack.
- Ageing of VRFB investigated.
- Analysis extended to multi-stack systems.

Competition of degradation mechanisms paradoxically leads to capacity retention

Discharge capacity



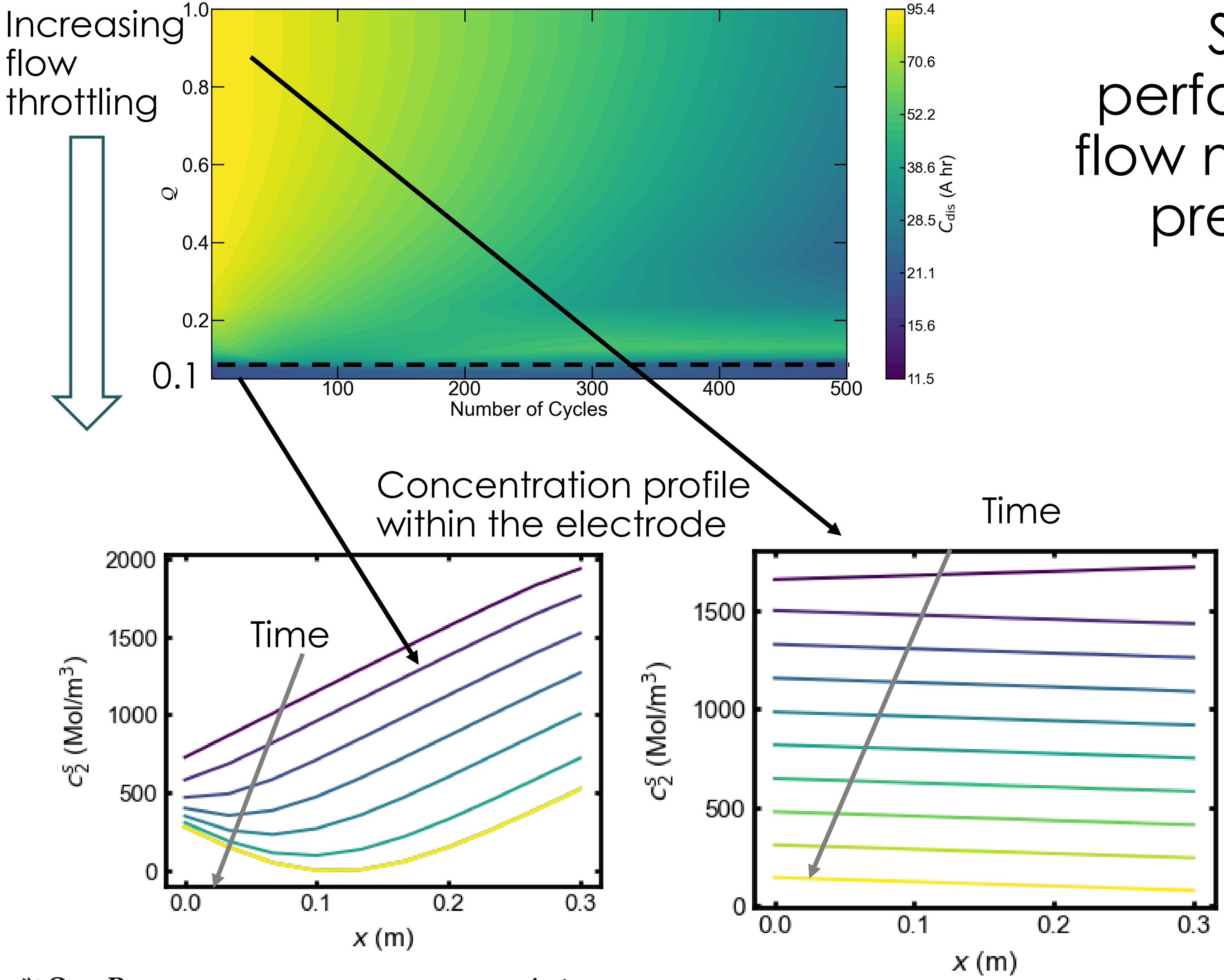
Ion concentration in electrode



- Ion imbalance drives capacity fade.
- HER parasitic current should lead to leftover V^{3+}.
- Literature shows ion crossover causes excess V^{2+}.
- Transition regime cancels out competing imbalance.

Skyllas-Kazacos, Maria, and Leesean Goh. "Modeling of vanadium ion diffusion across the ion exchange membrane in the vanadium redox battery." *Journal of membrane science* 399 (2012): 43-48.

Sharp drop off in performance at extreme flow maldistribution due to premature depletion



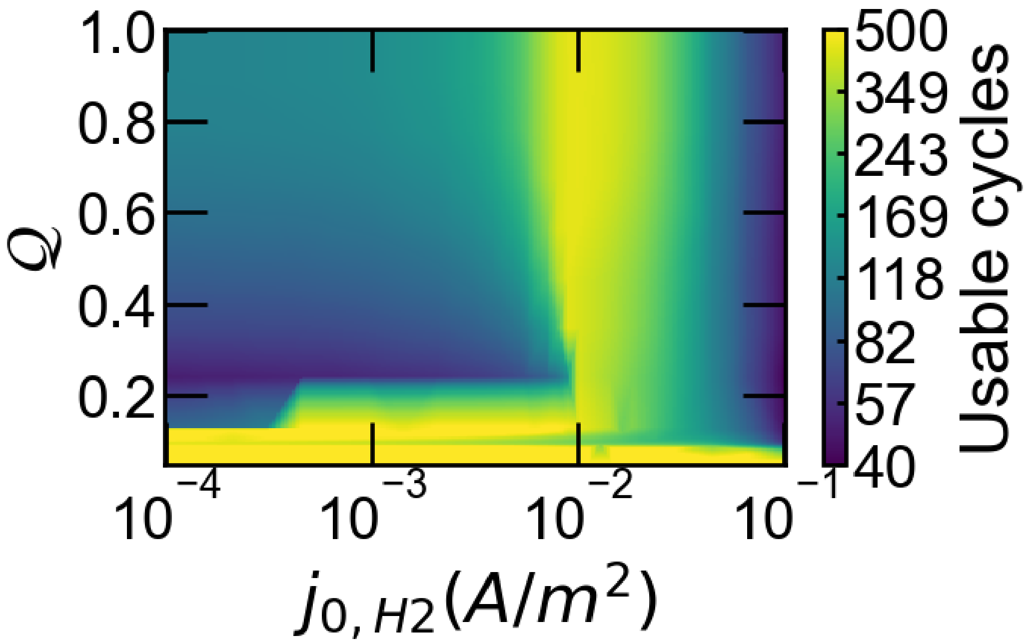
$j_{0,H_2} = 10^{-4}\ {}^{A}/_{m^2}$ Negligible HER

- One cell out of 37 has flow rate reduced.
- Low flow rate impedes active species supply in the electrode.
- Redox reactions consume faster than tank can replenish.
- Depletion in interior causes early voltage spikes.
- Premature voltage rise in one cell cuts the cycle off for the whole stack.

Unexpected regimes of enhanced capacity due to the interplay of the various degradation mechanisms

Full cell clogging

80% initial capacity retention

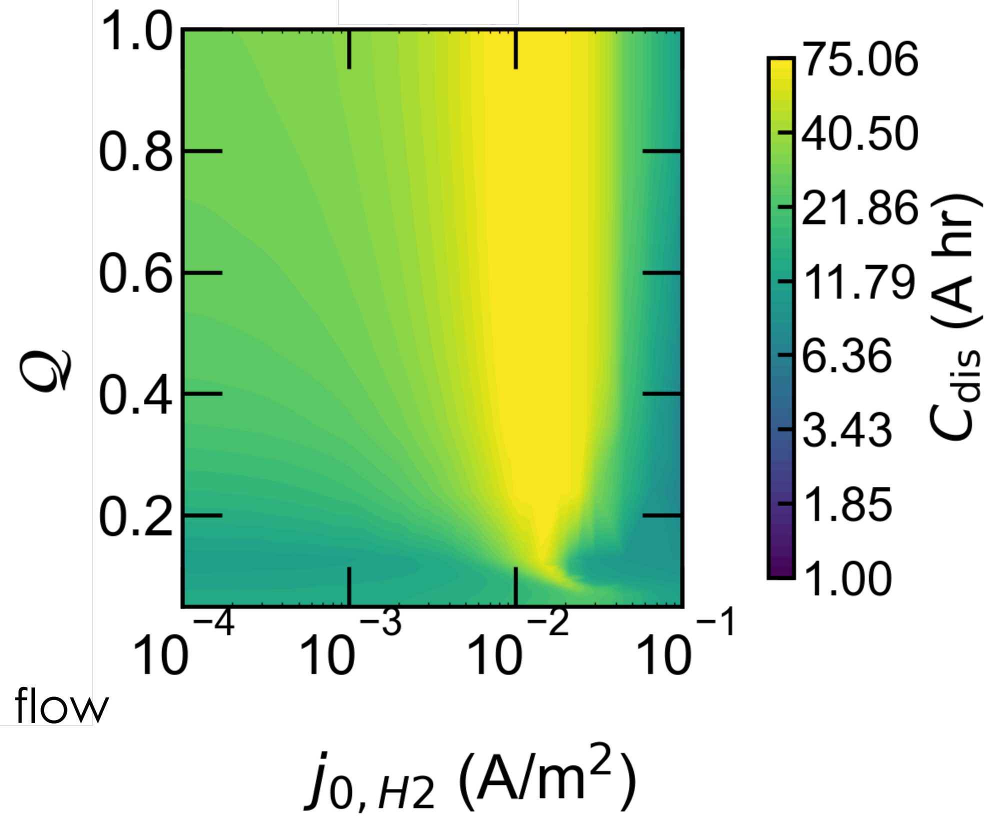


It should be noted that initial capacity can be significantly reduced at low Q

Positive half cell clogging

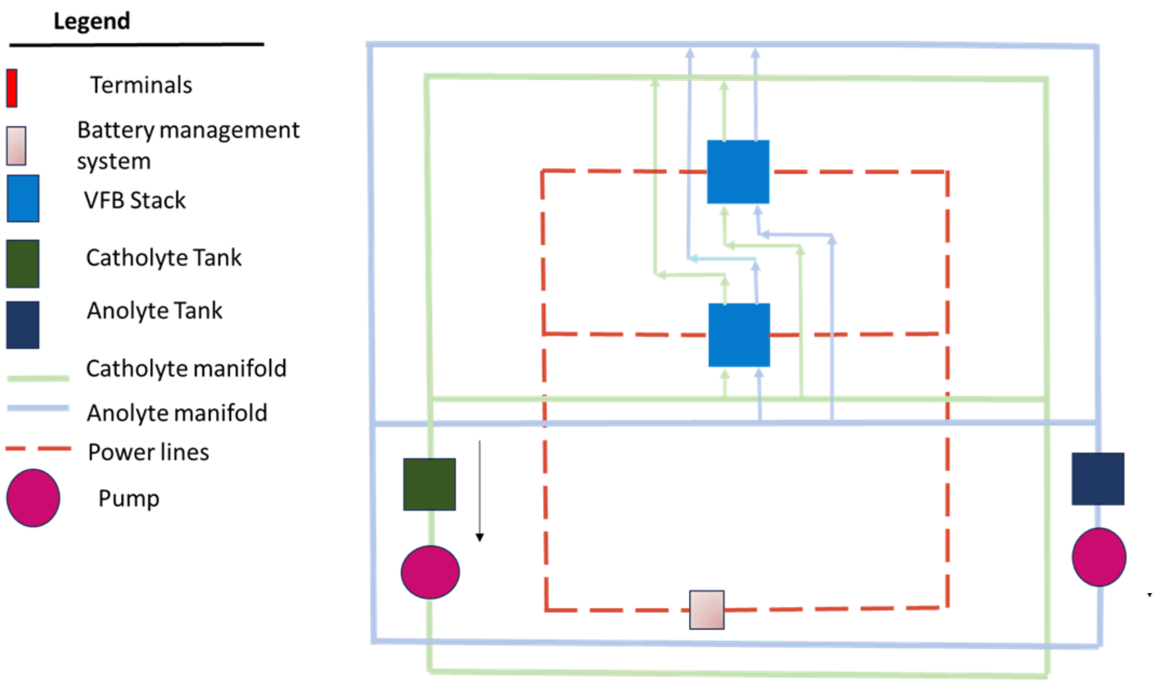
500 charge-discharge cycles

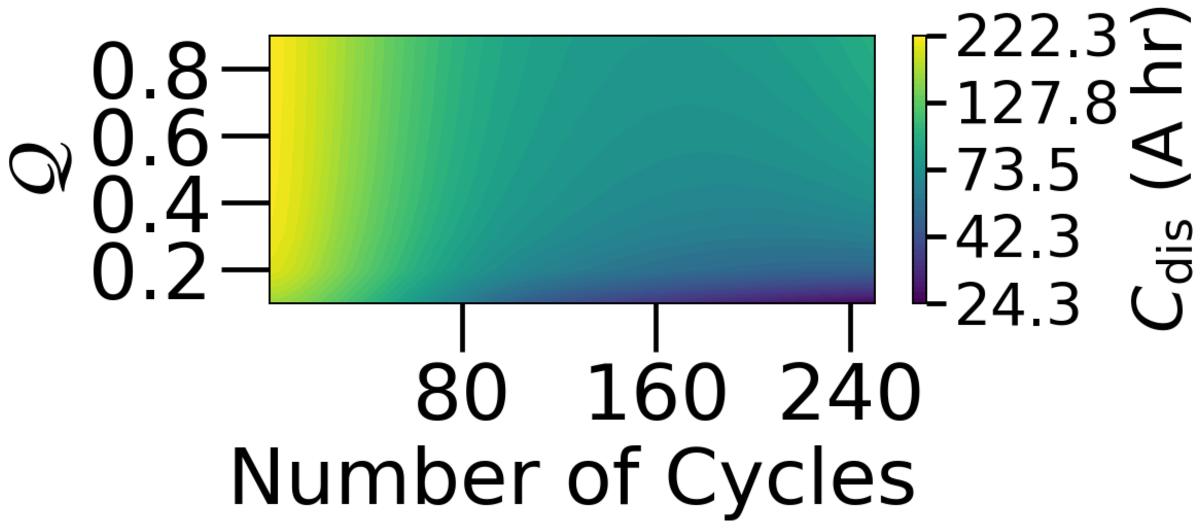
Increasing flow throttling



Manuscript under review in Energy Storage Materials

Analysis extended to multi-stack configuration





Impact of flow maldistribution is non-linear even with multiple stacks

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Cross-cutting collaboration: Integration with the Grid-C

Grid Systems Architecture team:

Renata Kimpara

Michael Starke

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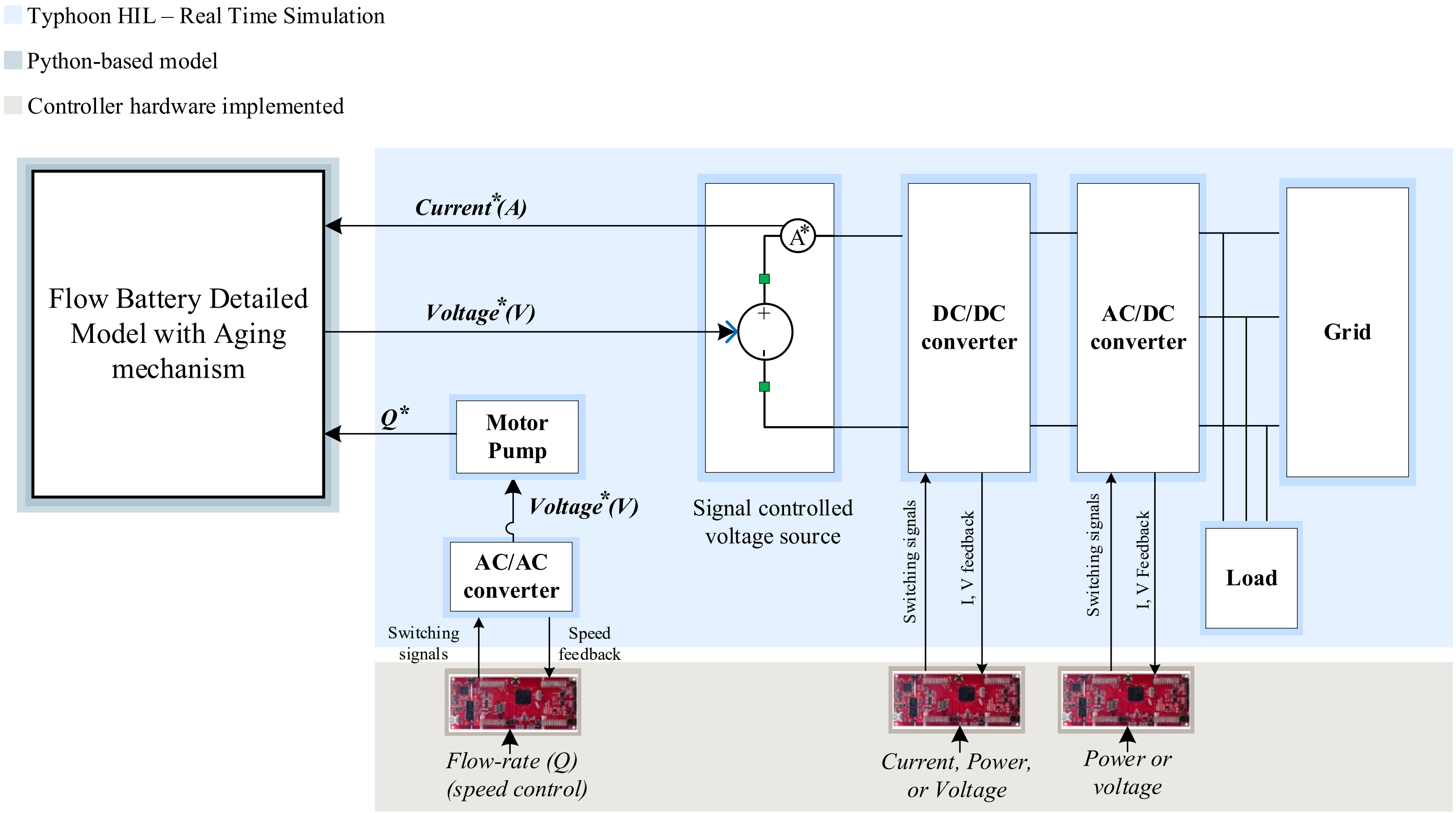
Planned next steps



Summary of Progress: FY 2026

- Incorporated hydrogen evolution and flow inhomogeneity into the VRFB simulation framework.
- Showed that crossover, HER, and clogging have a unique pair of vanadium species that are in limited supply and thus set the cycling of the battery.
- Identified multiple regimes of non-trivial discharge capacity evolution:
  - Crossover and HER can compete to paradoxically retain performance.
  - A throttled cell can dramatically slow down rate of capacity fade at the cost of low starting energy retention.
  - Reduced flow only to the half-cell shows improved performance at unexpectedly low cell throttling rates.
- Multi-stack results show that throttling single cell can hinder the performance of the whole system.
- Results presented at the ECS – Fall 2025 held in Chicago

Publications:

- **Johnson Dhanasekaran, Reed Wittman, Ethan Self, Sam Macchi and Srikanth Allu, "Impact of hydrogen gas and clogged cell on Vanadium Redox Flow Battery stack capacity" (In preparation -Energy Storage Materials)**

Next steps:

- Integration of the high-fidelity physics model with the Grid.
    - Communication *(ongoing)* and coupling *(upcoming)* of the physics and electrical grid simulation architecture
    - Electrical grid simulation –hardware in the loop for batteries developed by the GRID-C team at ORNL.

- Multi-stack system non-ideality impact on performance.
    - Flow delay between stacks *(ongoing)*
    - Shunt currents across stacks*(upcoming)*

- A physics informed ML architecture to dramatically reduce computational demand and increase feasibility of deployment.
    - Data generation for training. *(ongoing)*
    - ML implementation. *(ongoing)*

- Digital-Twin of VRFB for live forecasting. *(upcoming – long term goal)*

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Acknowledgements

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