Understanding the Impact of Hydrogen evolution and crossover on Performance of Vanadium Redox Flow Battery

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Project Profile

Topic: Flow Batteries, Large Scale Energy Storage

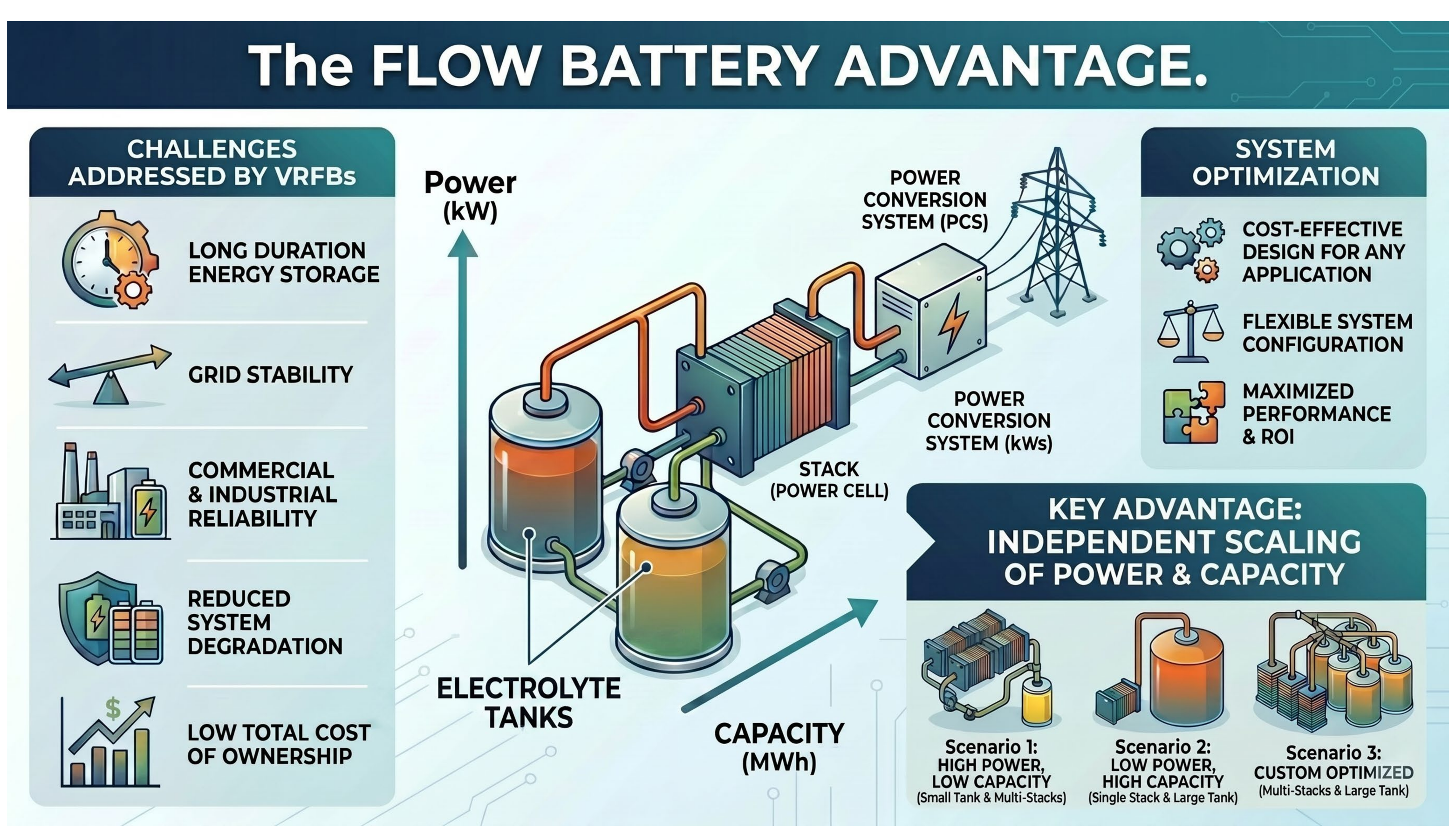
Vertical: Safety & Reliability

Strategic Pathway: Grow

Project start and finish: FY26-FY27

Problem

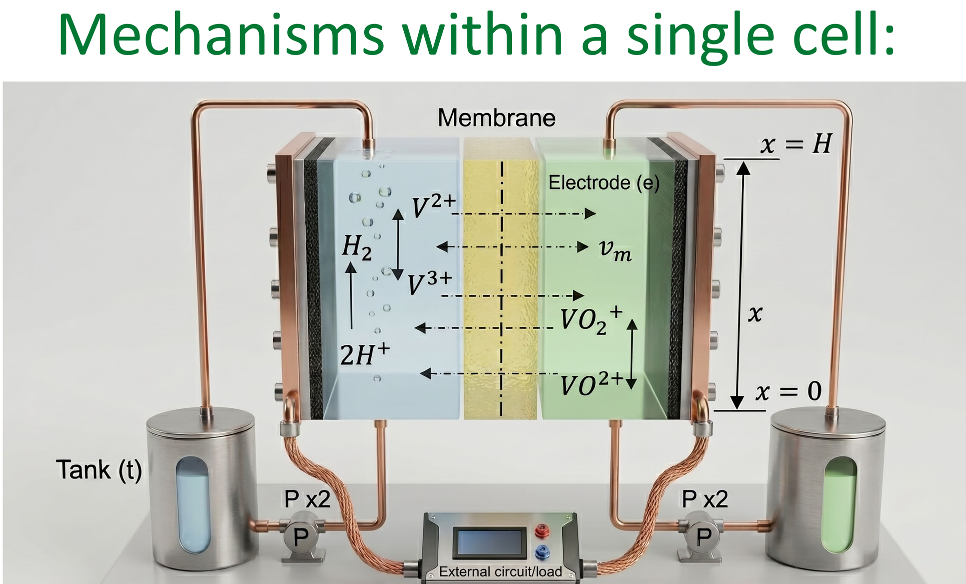
- Vanadium flow batteries (VFB) offer reliable long-term (excess of 6 hours) grid-scale energy storage (MW/MWh).
- VFB have significant cost and scalability advantage over lithium-ion batteries.
- Have been deployed on the field but many challenges into their operation remain such as hydrogen gas formation and flow maldistribution on the stack needs to be addressed.
- Simulation route is lucrative to identify performance bottlenecks over the expected very long lifetimes of VFB.



Approach

- Pseudo-two-dimensional electrochemical-flow first-principle cell model captures electrolyte reactions, mass transport, and fluid dynamics.
- Includes important degradations due to ion and electrolyte crossover and hydrogen evolution reaction (HER).
- Stack performance evaluated by assembling the cells into electrical series but parallel for electrolyte flow connection.
- Electrolyte flow in one half or full cell throttled to model design and manufacturing inefficiencies.

Mechanisms within a single cell:



HER: $I_{applied} = I_{redox} + I_{HER}$

Butler Volmer and Tafel equations for potentials.

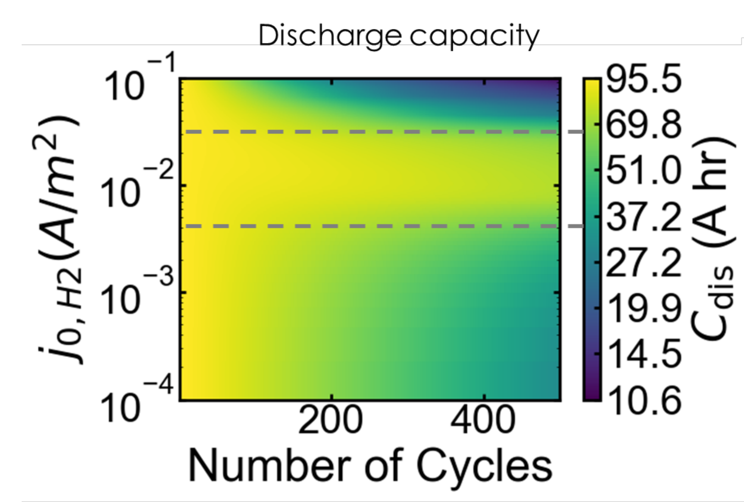
Impacts due to reduction porosity and electrolyte consumption included but shown to not be critical.

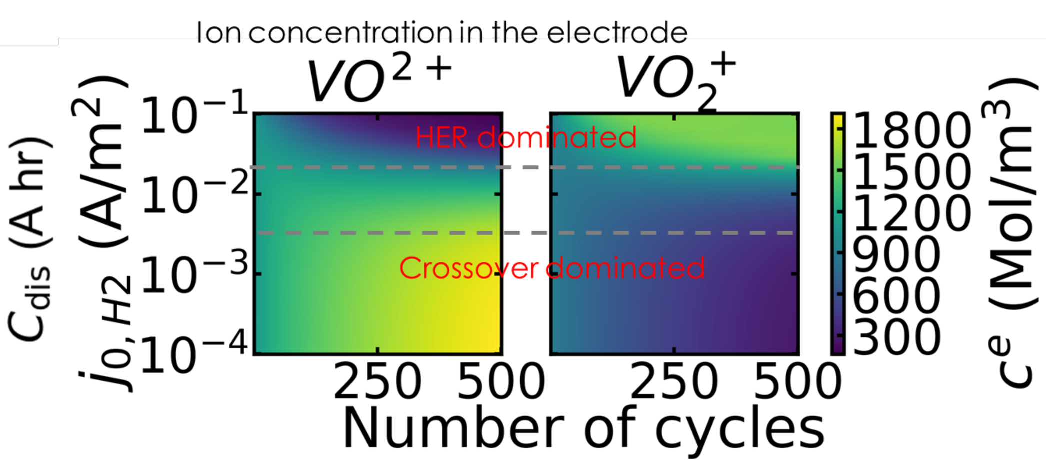
Mass transport: $V^e \frac{dc_i^e}{dt} = -Q^e H \frac{c_i^e}{dx} \pm \frac{I_{redox}}{zF} - A_m\left(\sum_i l_i n_i^{cross}\right)$; $V^t \frac{dc_i^t}{dt} = Q^t\left(c_{i|x=\mathrm{H}}^e - c_i^t\right)$

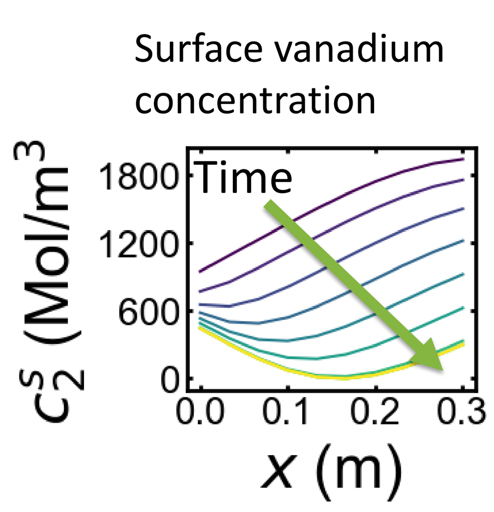
Crossover : $n_i^{cross} = \frac{k_i c_i^e}{D} + c_i^e v_m + \frac{z_i F}{RT} k_i c_i^e \frac{\Delta\Phi_1}{D}$; $\frac{dV^t}{dt} = \pm N v_m A_m$; $l_i \neq 0$

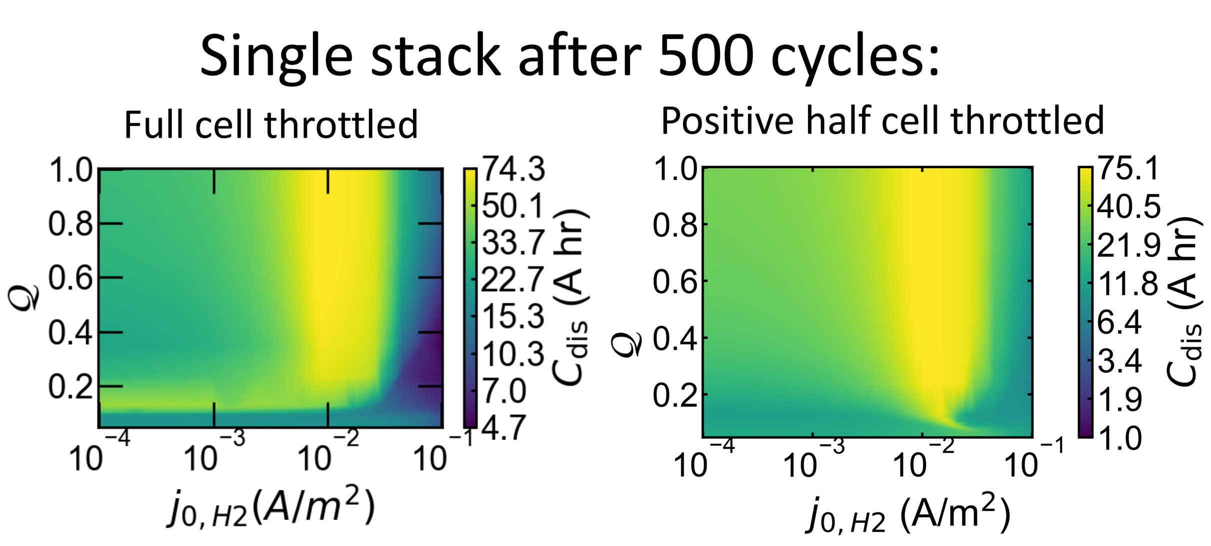
Results

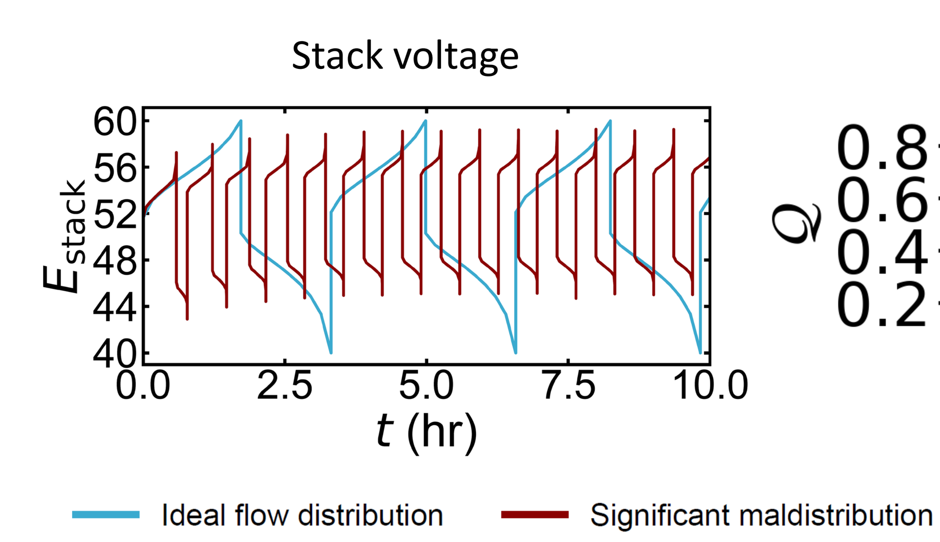
- Imbalance of vanadium ions drives discharge capacity loss, with the mechanisms driving in opposing directions.
- Reduced flow rate causes non-linear concentration profiles within the electrode and voltage spikes causing early cut-off thus dramatically affecting capacity fade.
- Smaller $\mathbb{Q}$ larger flow maldistribution.

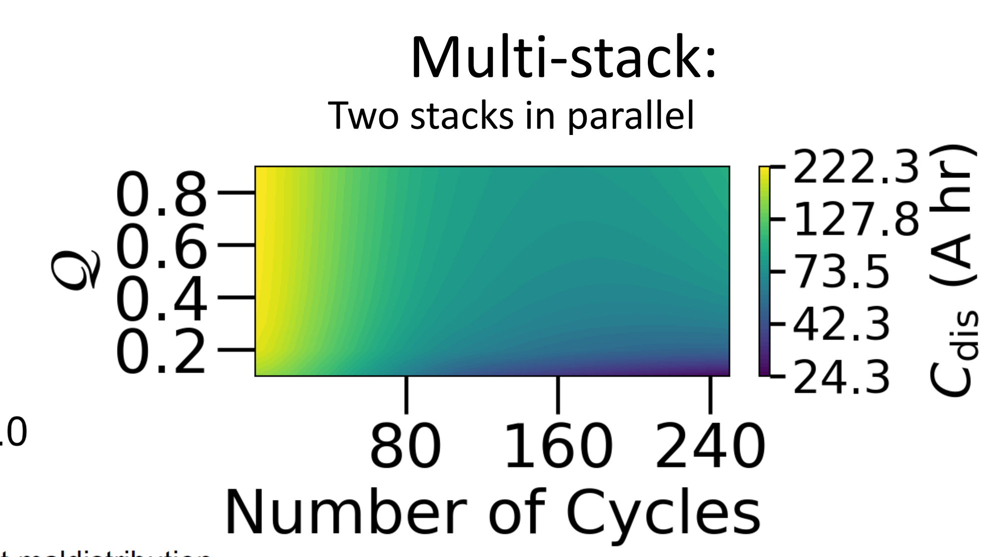












Conclusions & Impact

- First of a kind study on impact of the critical HER and flow maldistribution on VFB stack performance.
- Identified multiple novel phenomena of VFB discharge capacity evolution that will influence their operation.
- For example, mild HER can potentially improve battery life.
- Produced a phase diagram of discharge capacity over the various non-idealities.
- Results presented at ECS Fall 2025 (Chicago) and manuscript is under internal review.

Future Directions

- Deploying MW/MWh multi-stack VFB system to provide support to real-world grid deployment.
- Accelerated AI models can be used to gain insights during critical operational envelope.
- Integration are planned with controller Hardware-In-Loop of the electrical grid In collaboration with the GRID-C team (at ORNL).
- Flow delay and shunt current between the various stacks will be incorporated to capture operational non-ideality.

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