



# Near Real Time Diagnosis and Prognosis Framework for Redox Flow Batteries

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**Jie Bao**

Vince Sprenkle, Yunxiang Chen, Yucheng Fu,  
Emily Saldanha, Chao Zeng, Soowhan Kim,  
Ed Thomsen, Peiyuan Gao, Vish Viswanathan,  
Alasdair Crawford, Amanda Howard, Wei Wang

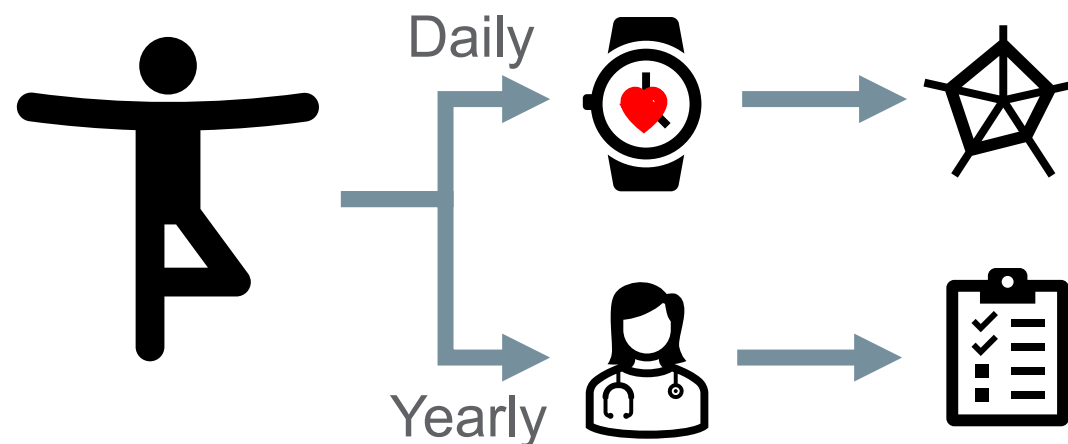


PNNL is operated by Battelle for the U.S. Department of Energy



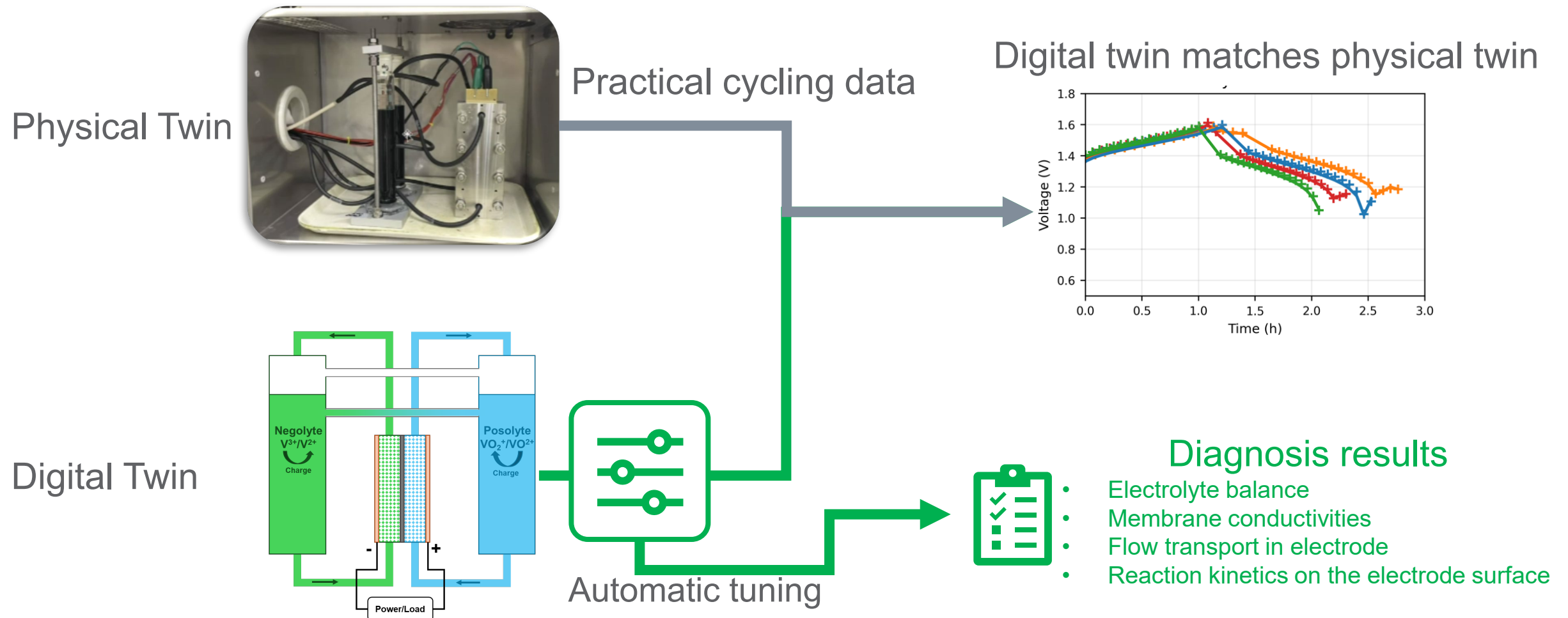
# Battery State of Health Diagnosis

- Regular cycling or practical duty-cycle testing can indicate approximate capacity and efficiency.
- However, these tests cannot reveal the underlying causes or degradation mechanisms.
  - Electrolyte balance → affects capacity
  - Membrane conductivity → affects ohmic resistance
  - Mass transport in the electrode / flow field → affects concentration resistance
  - Reaction kinetics at the electrode surface → affects activation resistance
- Reference performance tests (RPTs) can provide a more detailed assessment of battery state of health (SOH).
- However, they are often limited by time, cost, and operational complexity.
  - RPT: Electrochemical Impedance Spectroscopy (EIS), Pulse current test, Polarization test, Deep charging/discharging test, etc.
  - For large-scale battery systems, some RPT methods may be impractical or infeasible.



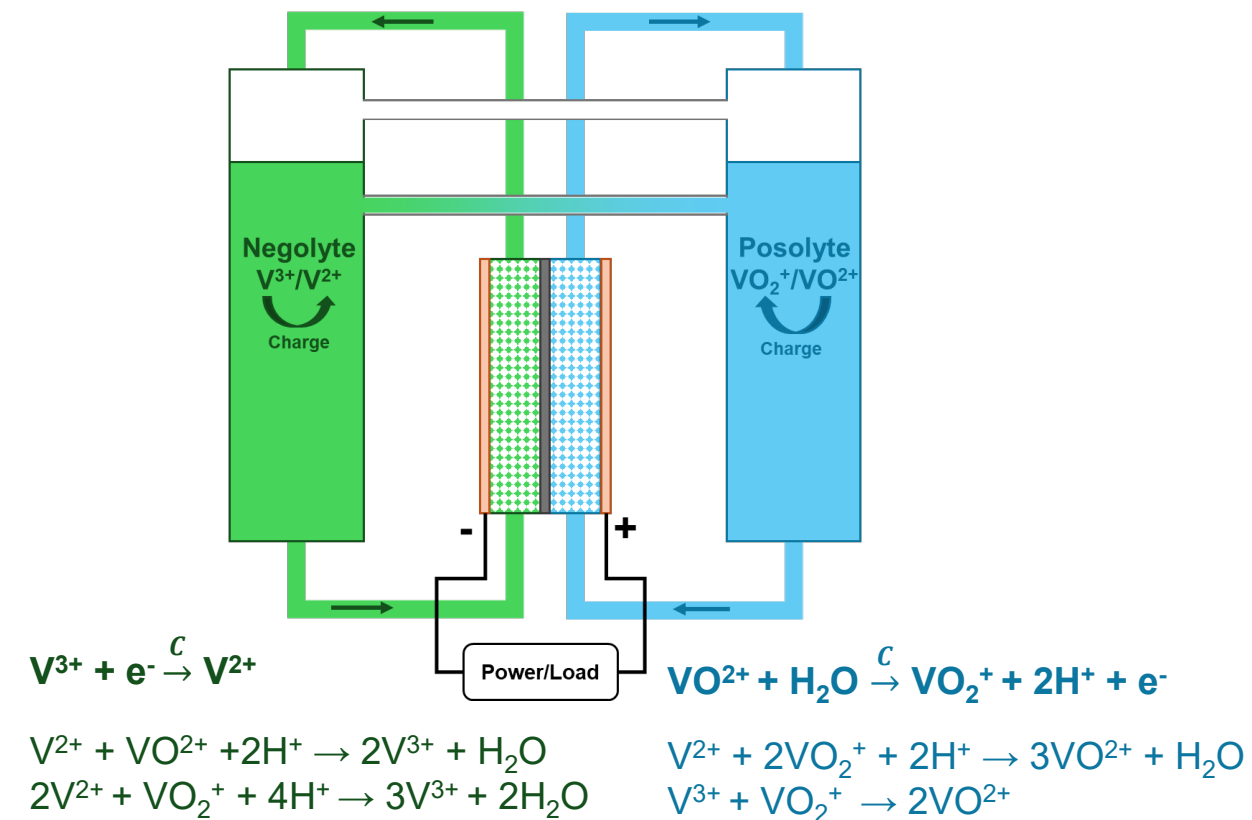
# Digital Twin for Diagnosis

- A digital twin can be used for real-time diagnosis.
  - The digital twin can automatically tune material properties and battery parameters so that the predicted cell performance matches the actual battery behavior..



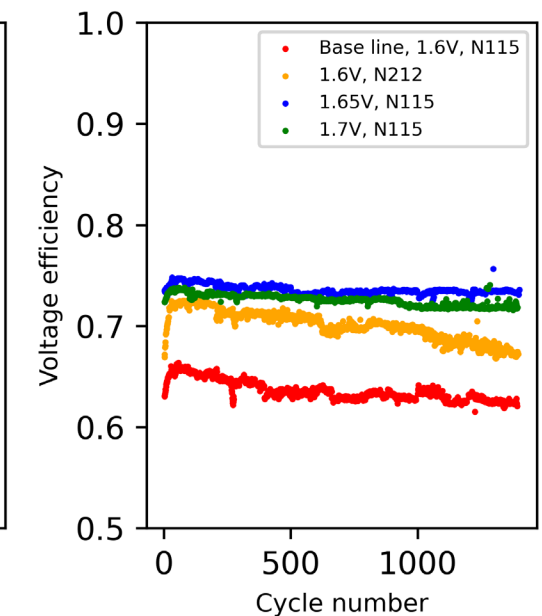
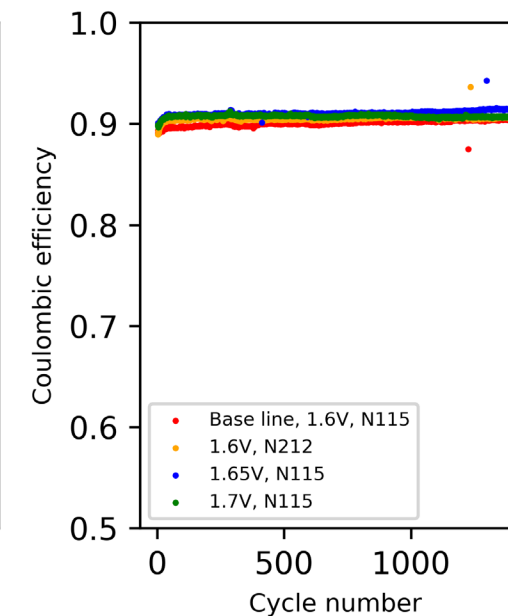
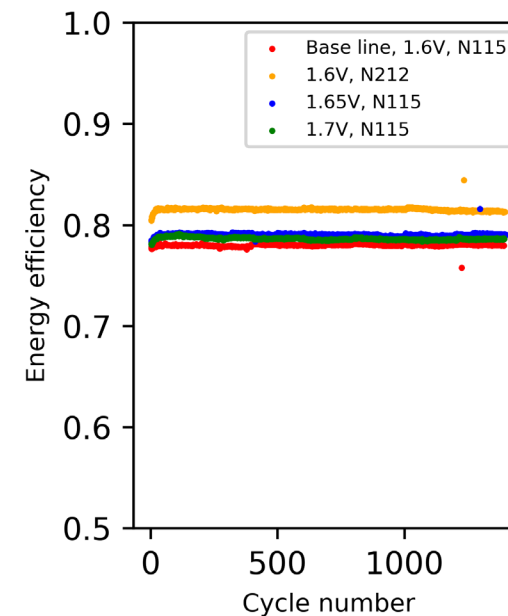
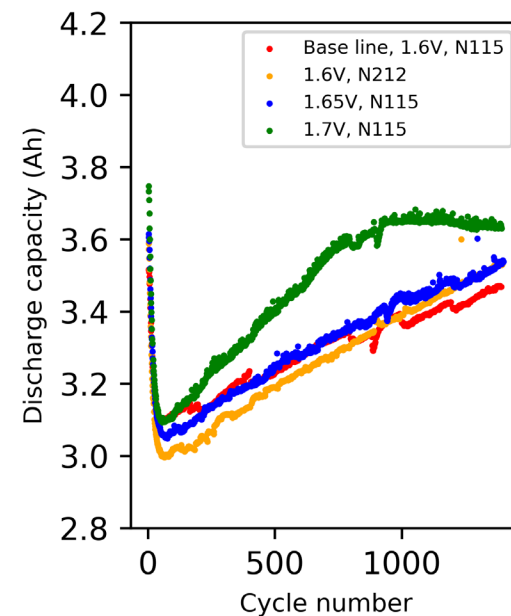
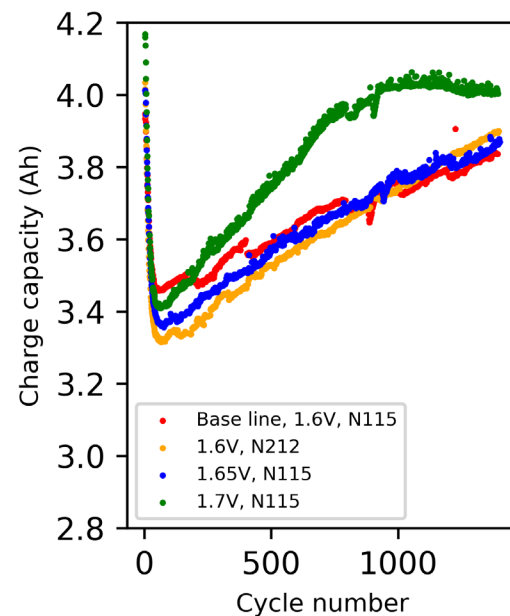
# Does this Digital Twin Concept Actually Work for Redox Flow Batteries?

- Validation study
  - Physical twin
    - 27 cm<sup>2</sup> active area electrode for both sides
    - 105 ml electrolyte each side
    - Initial concentration 1.6 M on each side
    - Liquid bridges configuration
    - Test conditions:
      - 1.6 V cut off voltage, N115 membrane
      - 1.6 V cut off voltage, N212 membrane
      - 1.65 V cut off voltage, N115 membrane
      - 1.7 V cut off voltage, N115 membrane
  - Implement the traditional diagnosis every 200 cycles
    - EIS, pulse current test, polarization test
  - Evaluation: Compare traditional diagnostic results with digital twin real-time diagnostic results



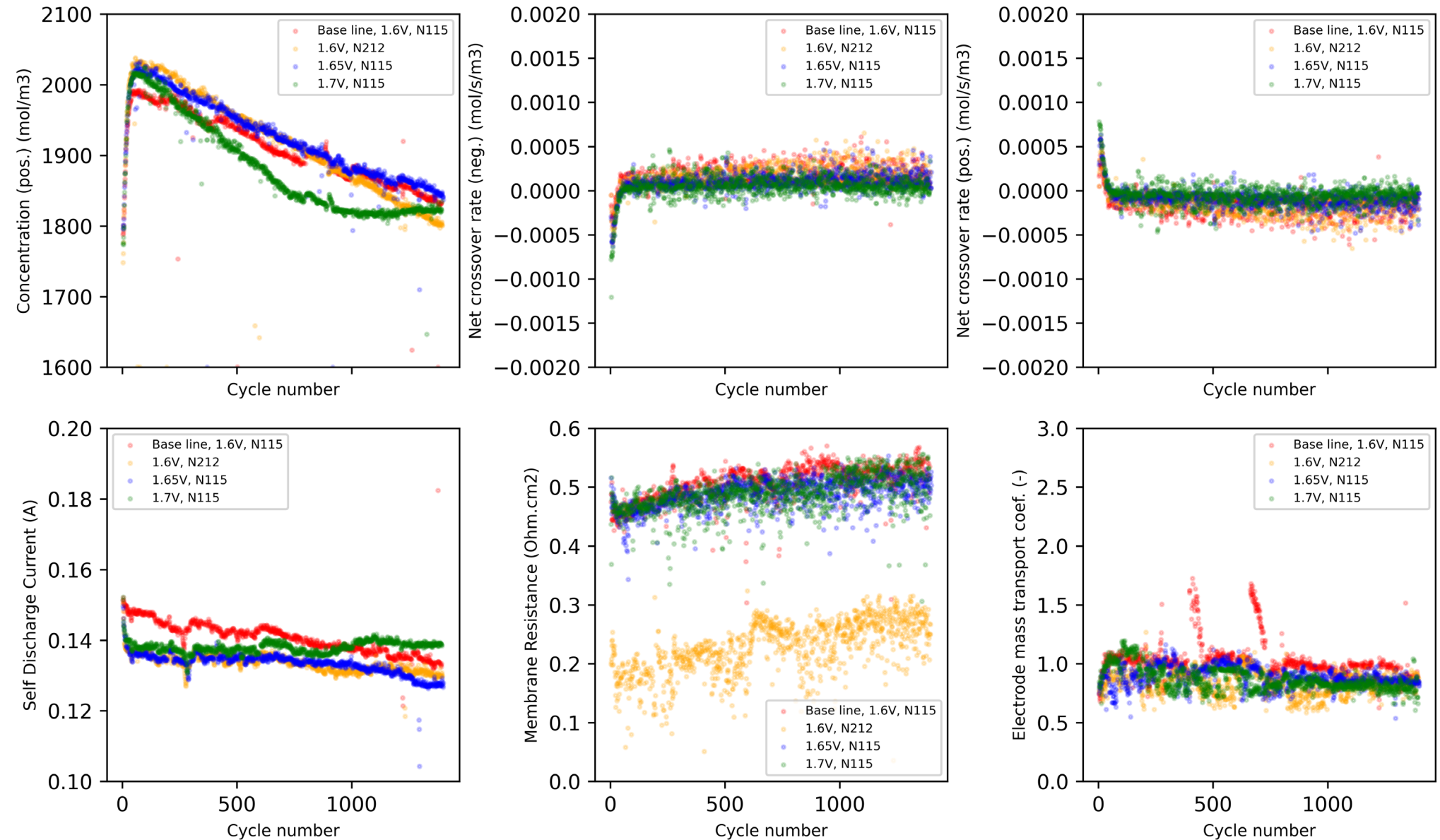
# Experiment Results for Diagnosis

- The theoretical capacity is 4.503 Ah.
- All the 4 cases show similar trend of degradation.
  - Rapid decrease of capacity at beginning, and then gradually recover



# Diagnostic Results from Digital Twin

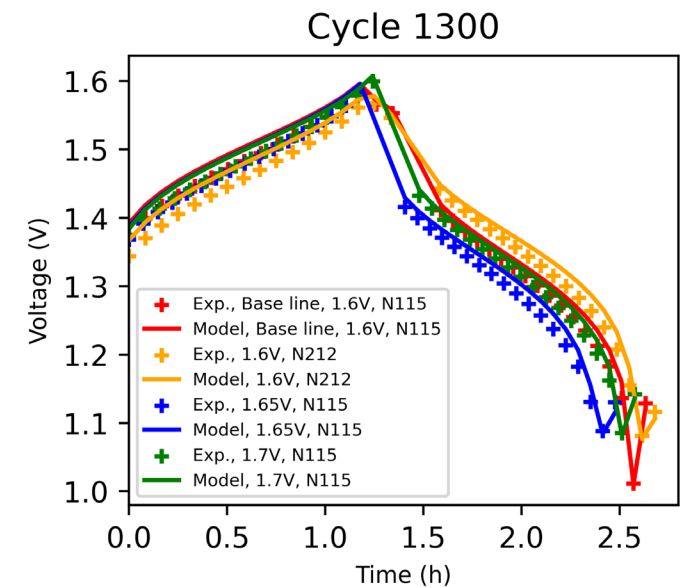
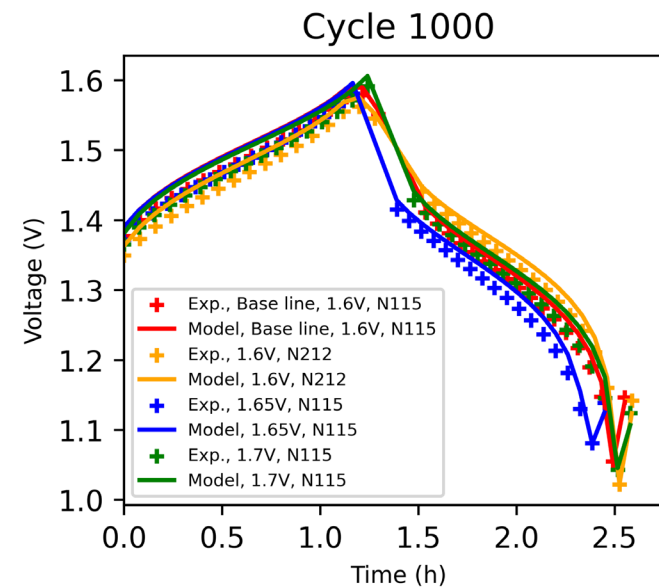
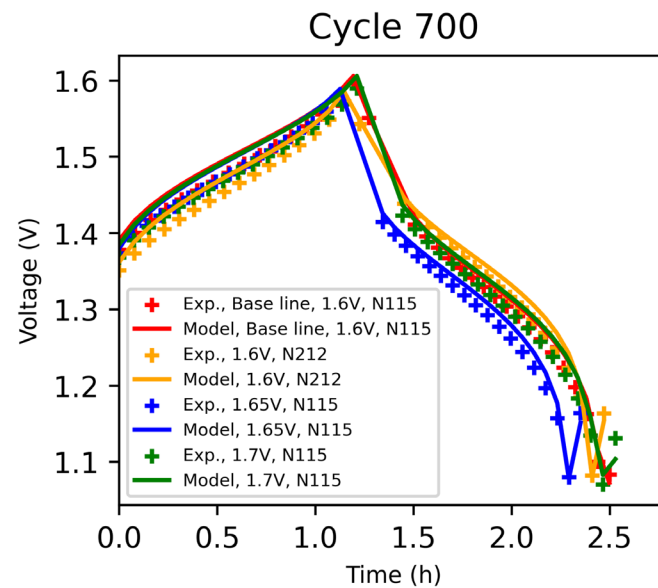
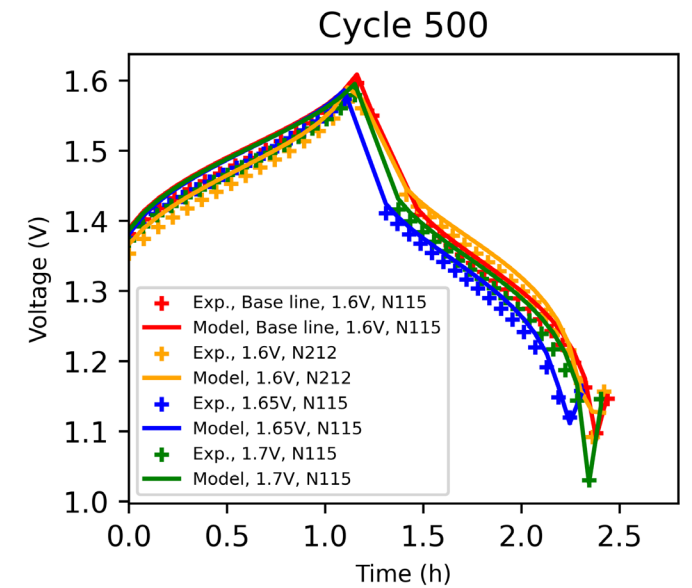
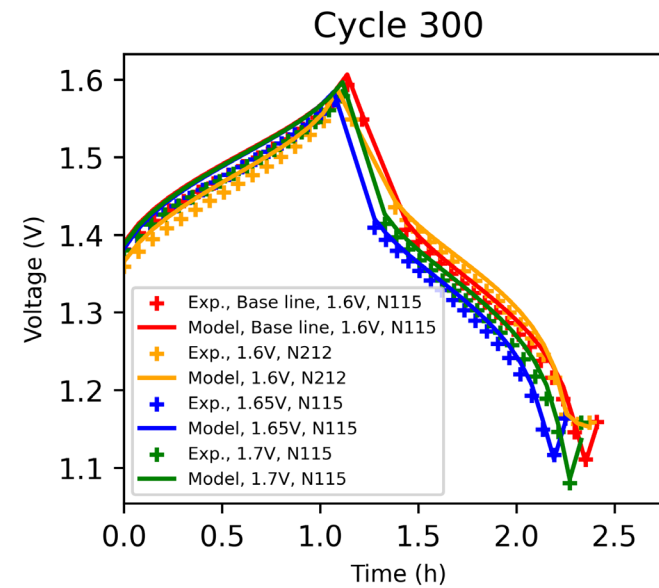
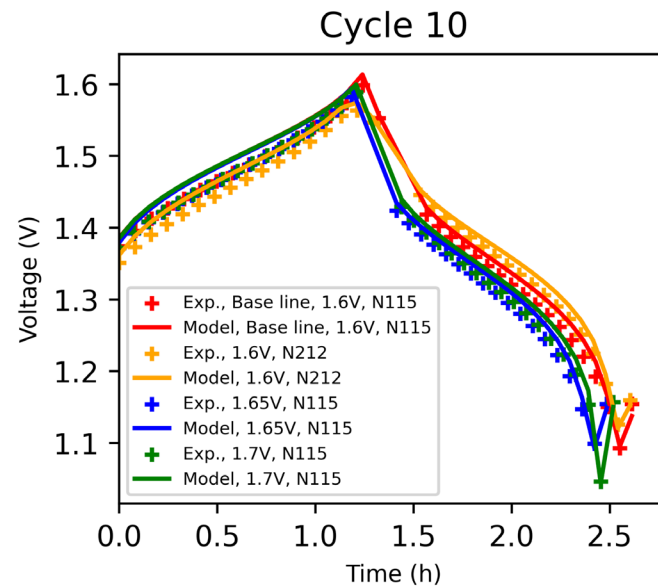
- The Digital Twin is based on a physical-based flow battery modeling framework **EZBattery**
- Strong active-species crossover causes rapid capacity fade during the first 50 cycles.
- The liquid bridge gradually rebalance the active species to recover the capacity.
- The liquid bridge also increases self-discharge current and reduces coulombic efficiency.



# Diagnostic Results from Digital Twin

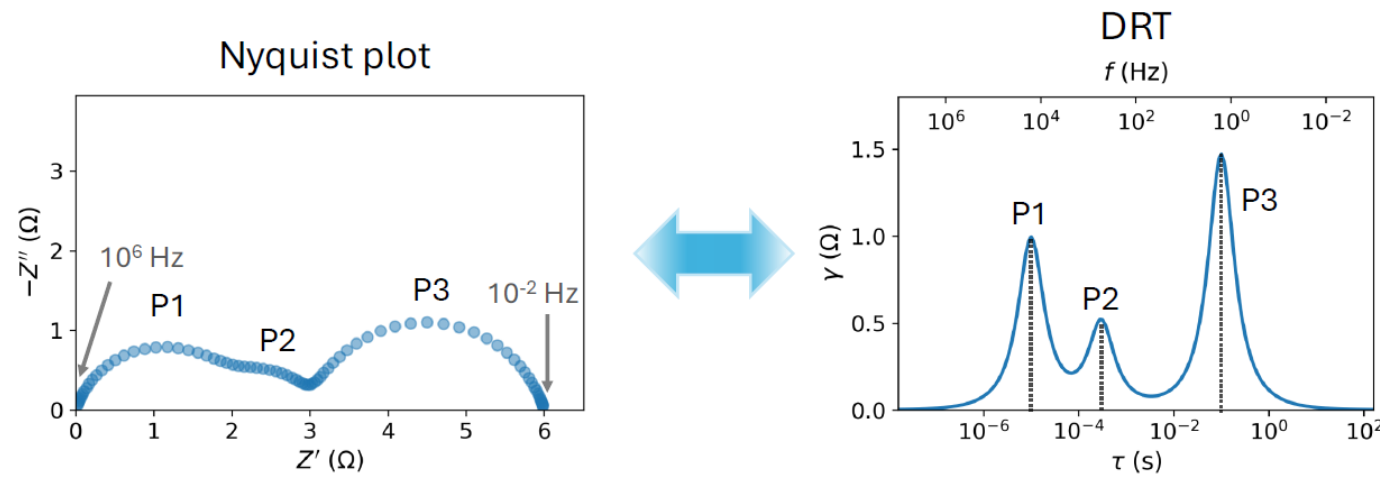
## Validations

- The diagnostic results enable the physics-based model **EZBattery** to predict cell performance in close agreement with the experimental data.
- The averaged error is lower than 20 mV.

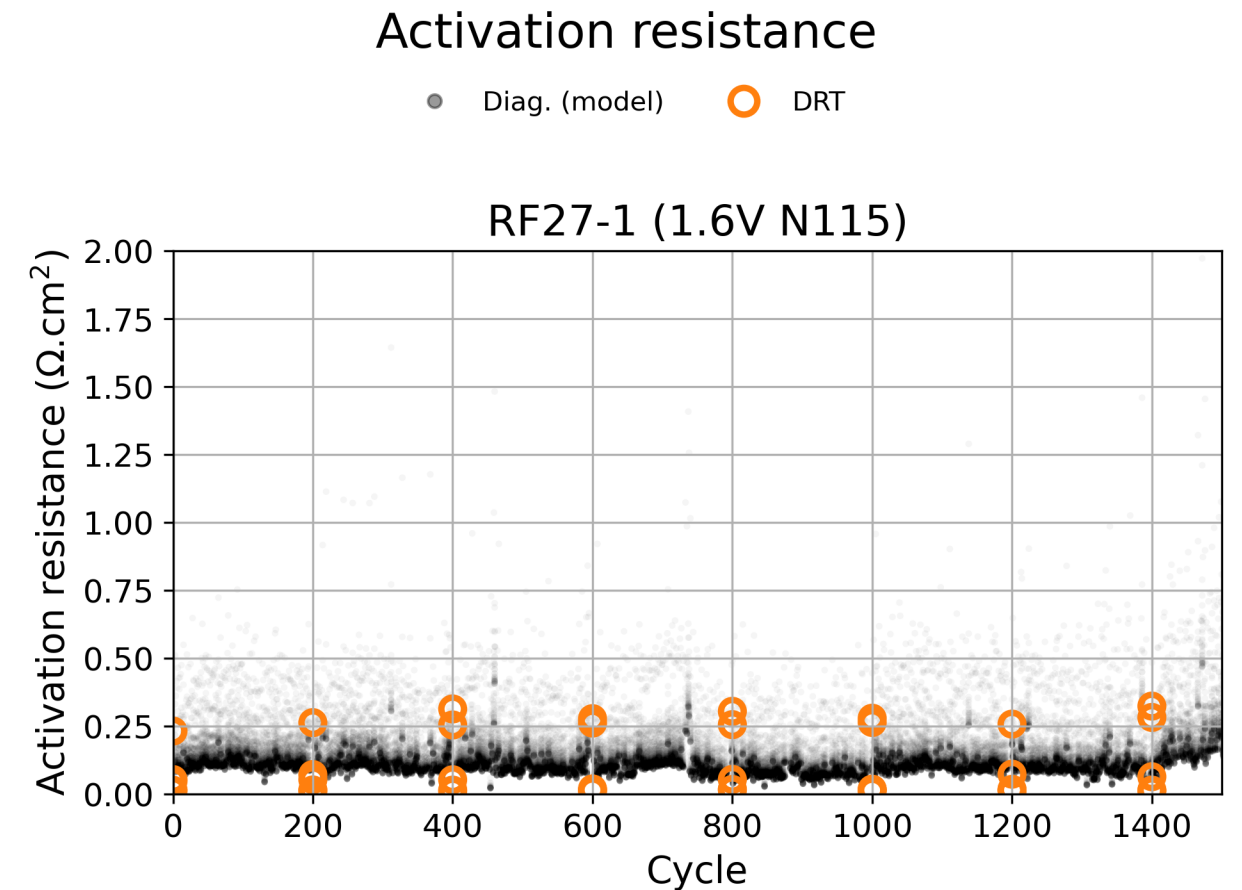


# Diagnostic Results from Digital Twin

- Validation with the traditional diagnostic results



- DRT: distribution of relaxation time
- DRT peaks indicate processes with different relaxation times.
- The RPTs were implemented at SOC 0, 25, 50, 75, 100%

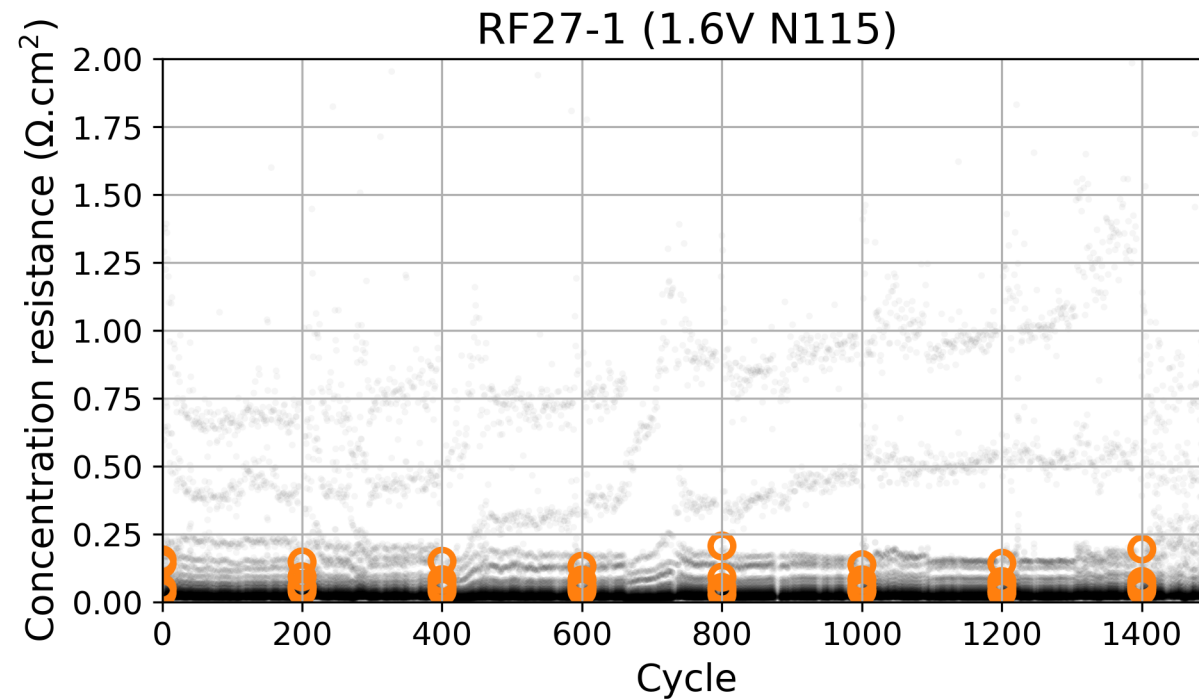


# Diagnostic Results from Digital Twin

- Validation with the traditional diagnostic results

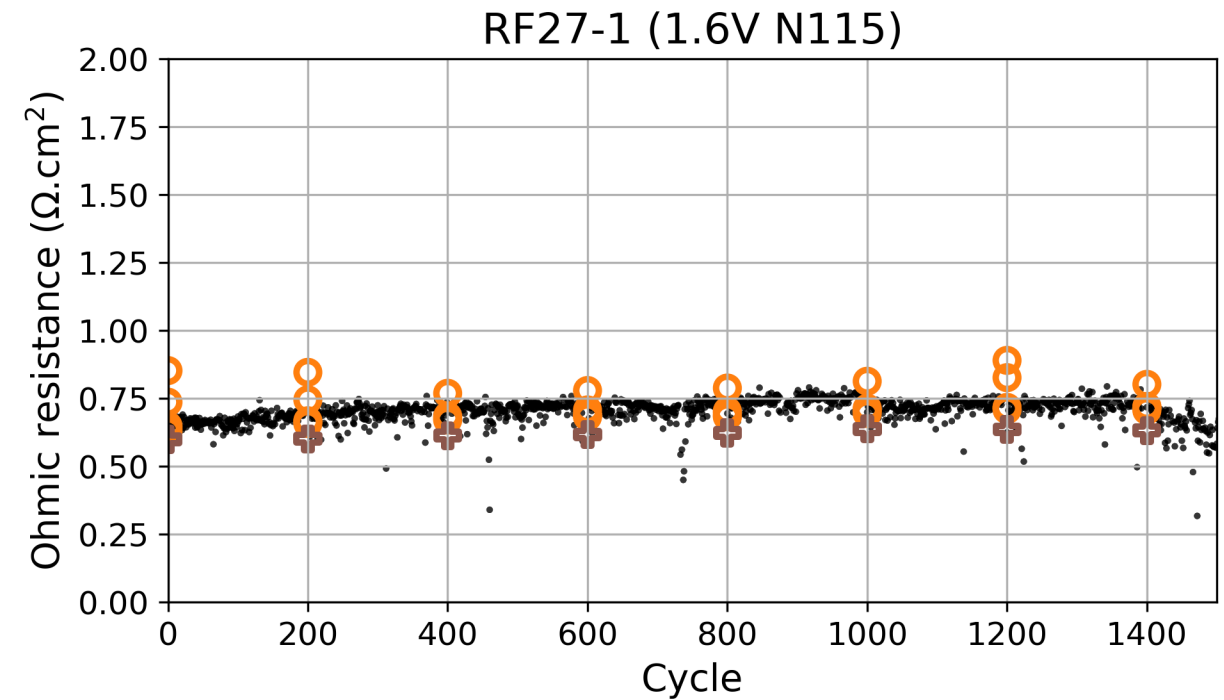
Concentration resistance

● Diag. (model) ○ DRT



Ohmic resistance

● Diag. (model) ○ DRT + HFR

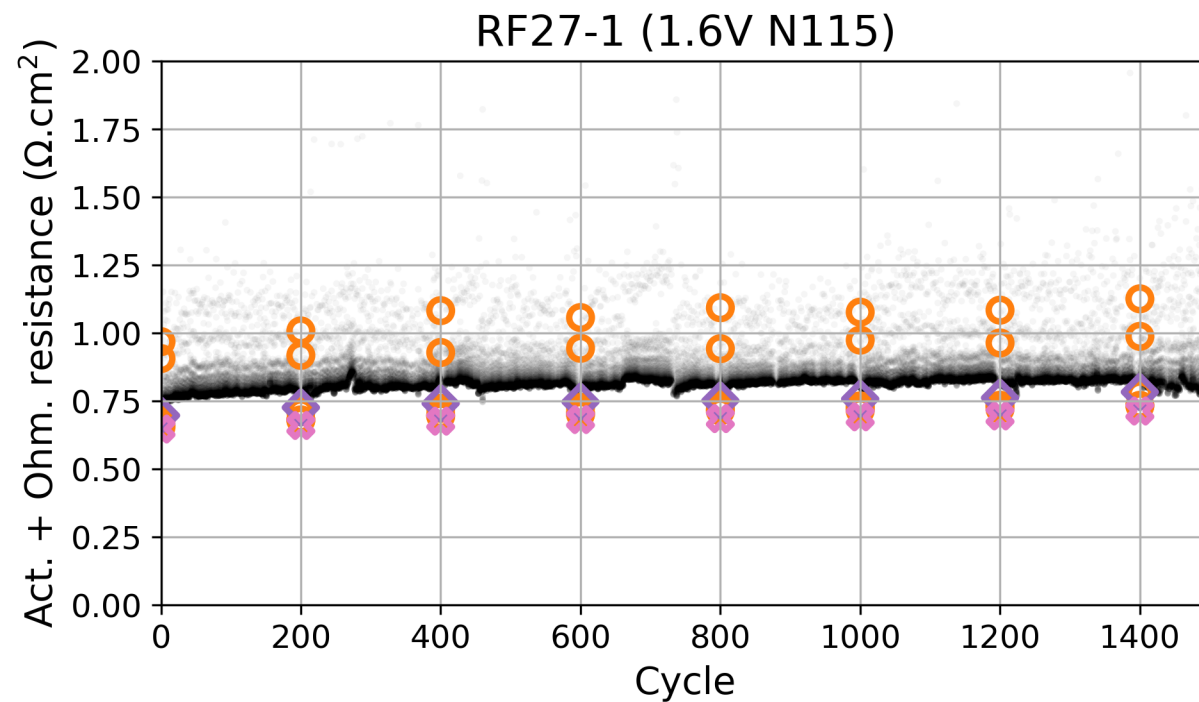


# Diagnostic Results from Digital Twin

- Validation with the traditional diagnostic results

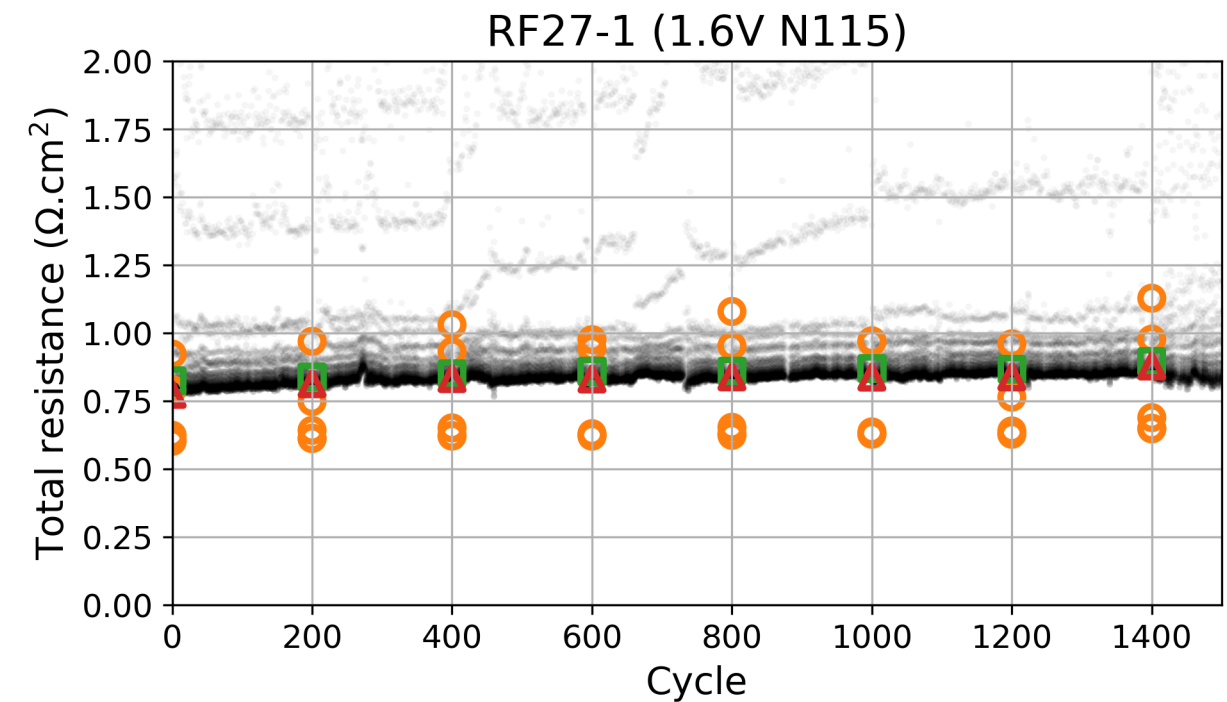
Act. + Ohm. resistance

● Diag. (model) ○ DRT ◇ R Impedance ✕ R Pulse



Total resistance

● Diag. (model) ○ DRT □ R Pol,D ▲ R Pol,C

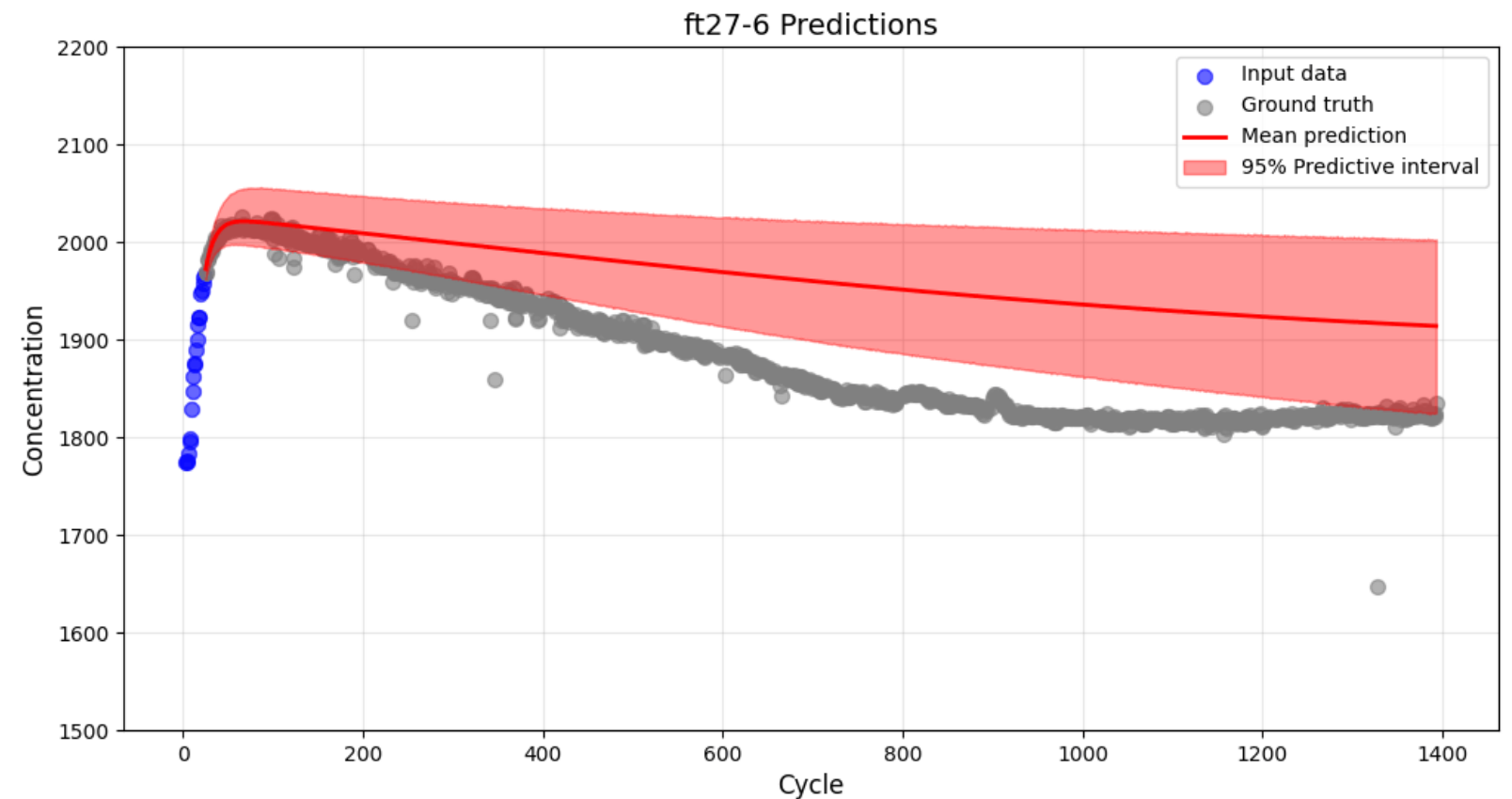


# Prognosis: long-term prediction using early-cycle data



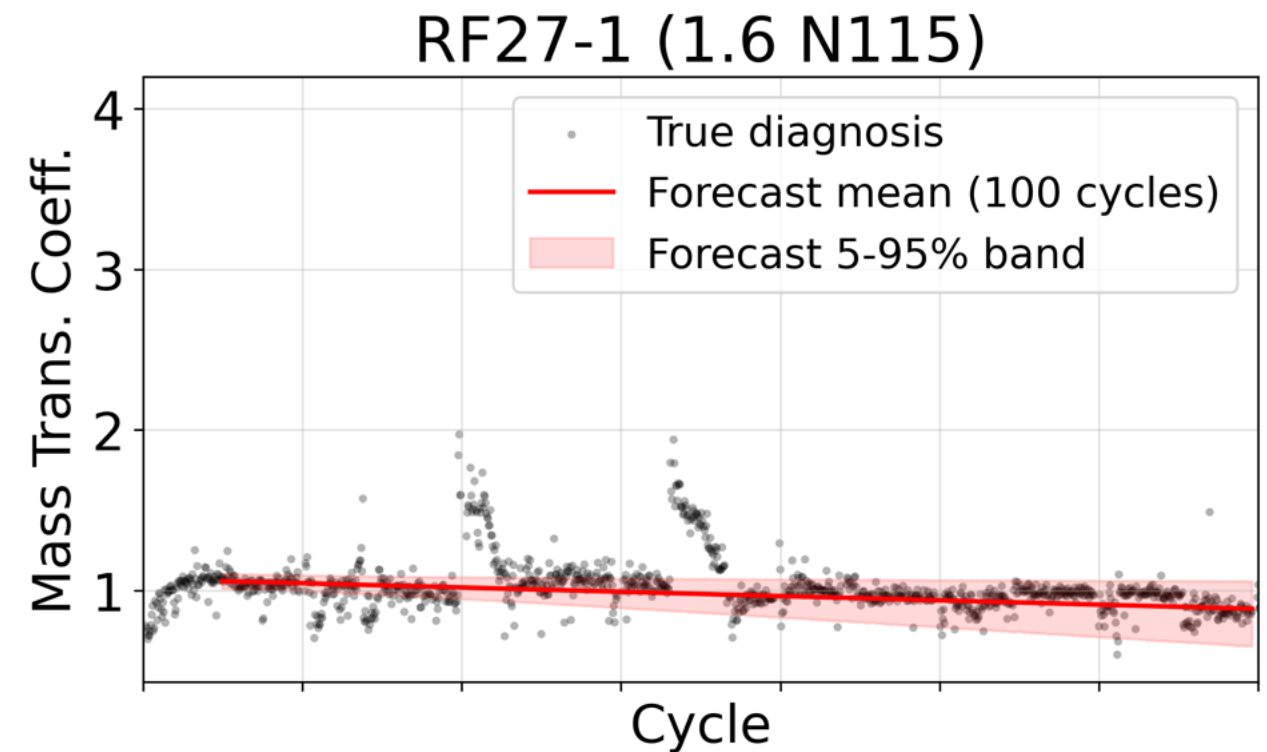
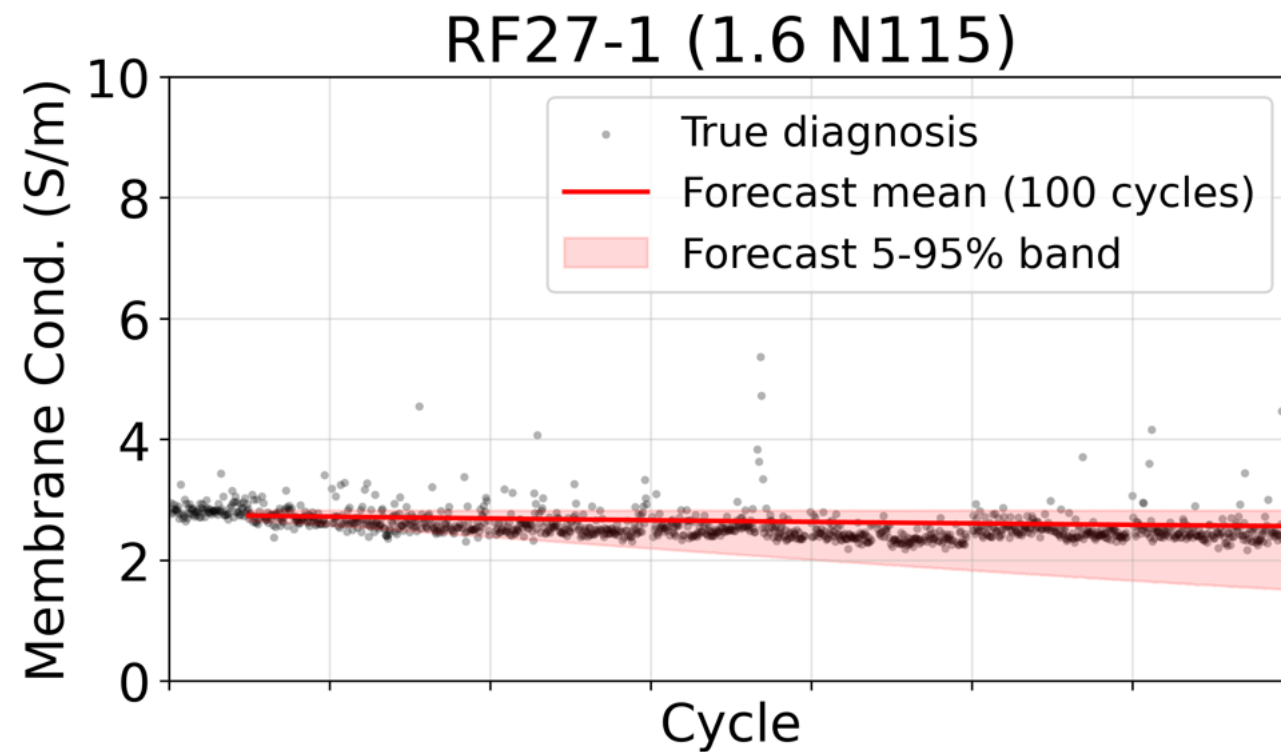
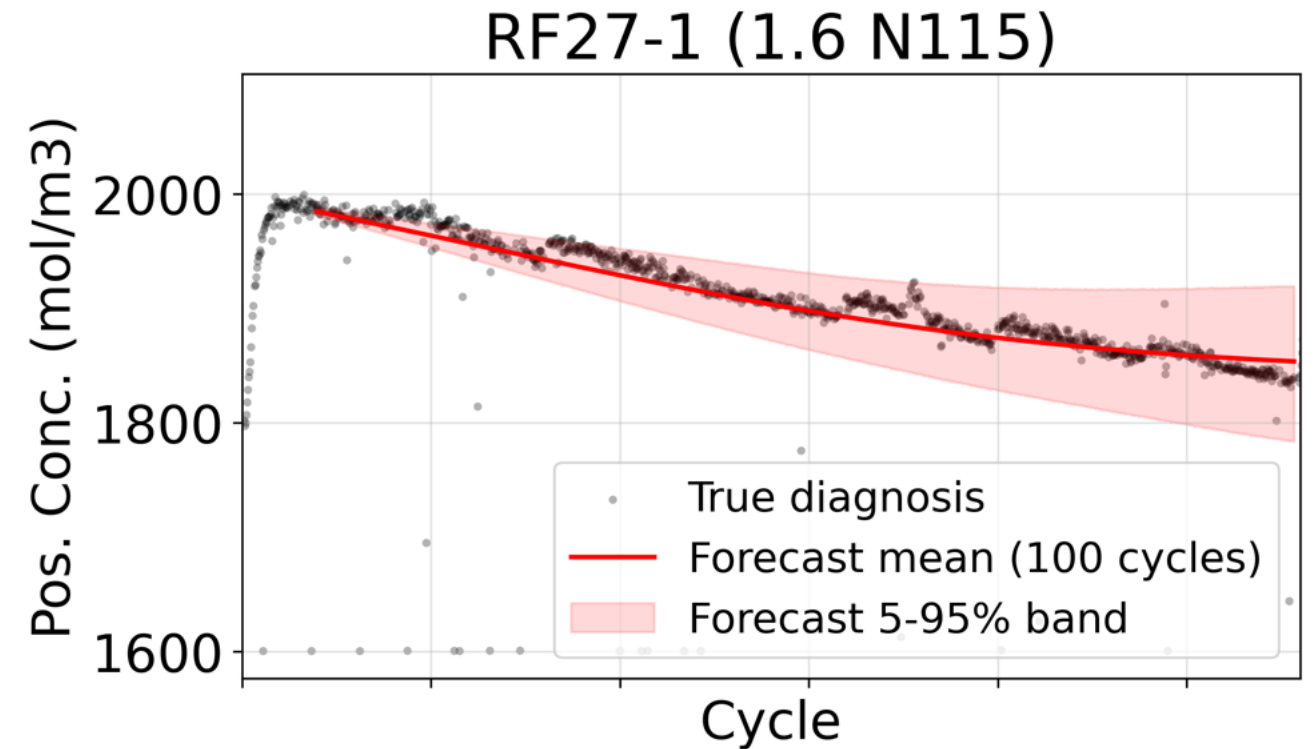
- Can the First 100 Cycles Be Used to Forecast Cell Performance over the Next 1,000+ Cycles?

- **Functional-form selection:** Each parameter is independently described using a functional form that reflects its observed degradation trend.
- **Bayesian inference:** Parameters are estimated in PyMC through MCMC sampling with informative priors.



# Prognosis Validations

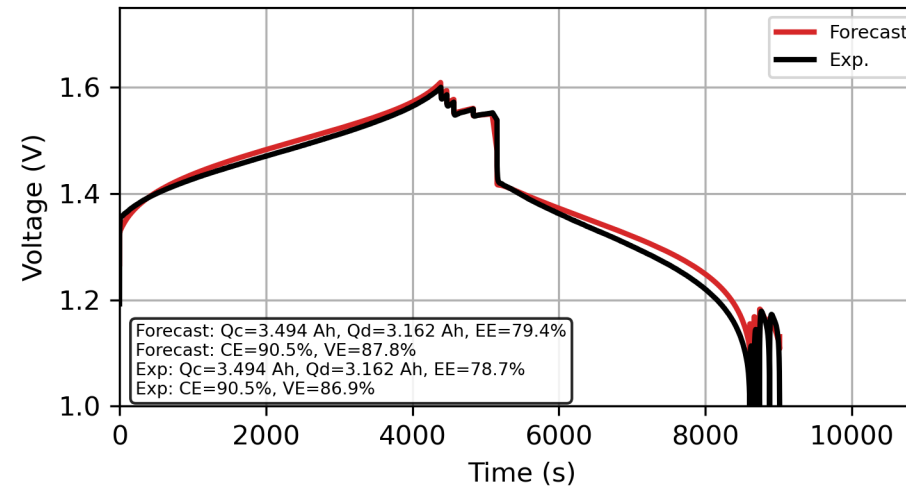
- Diagnostic results from the first 100 cycles are used to forecast the degradation of cell properties and model parameters over the next 1,300 cycles.



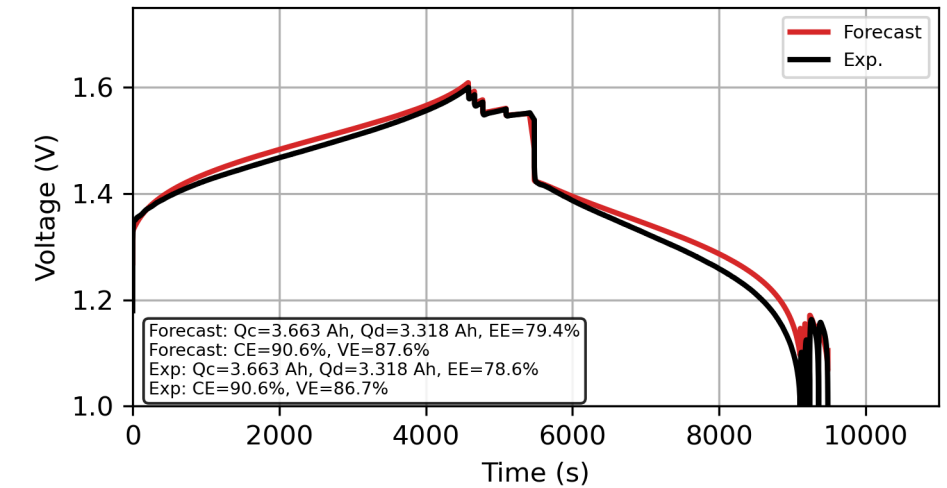
# Prognosis Validations

- The forecasted battery properties and parameters are used to predict cycling performance in **EZBattery**.
- The predicted cycling performance is compared with experimental measurements at cycles 150, 650, 1000, and 1300.

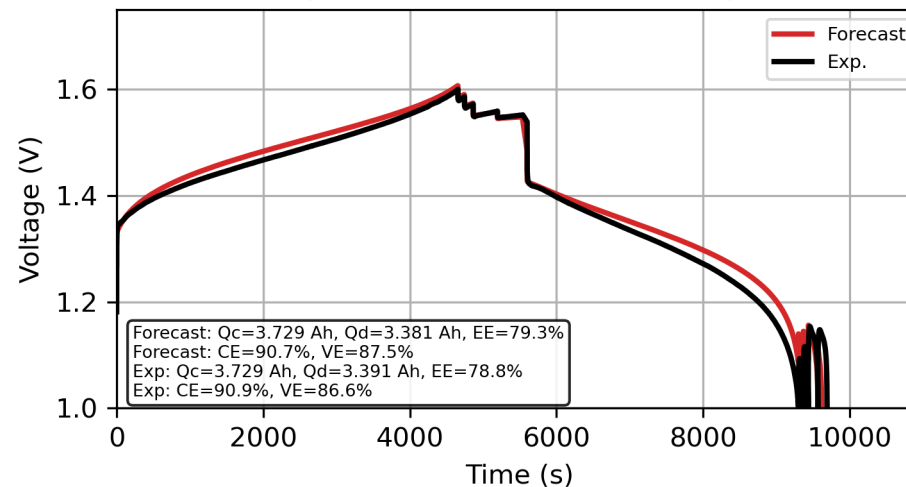
Cycle 150: Forecast vs. Exp.



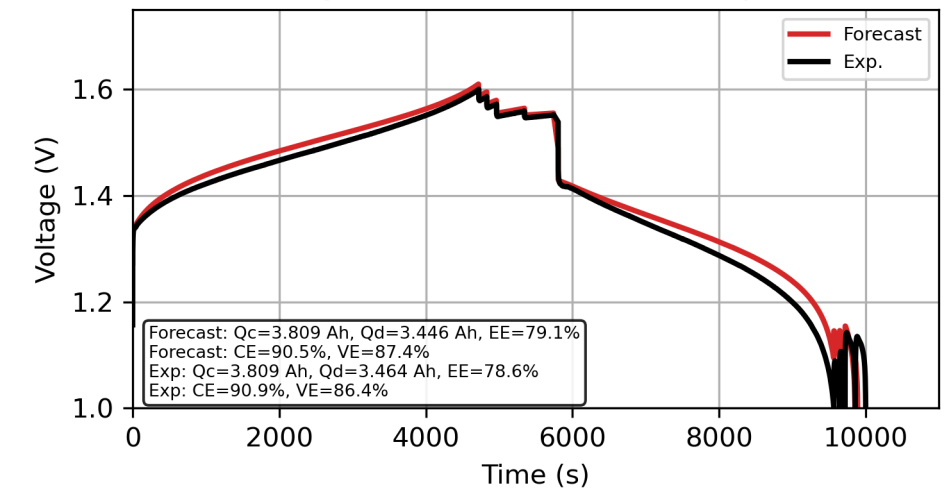
Cycle 650: Forecast vs. Exp.



Cycle 1000: Forecast vs. Exp.

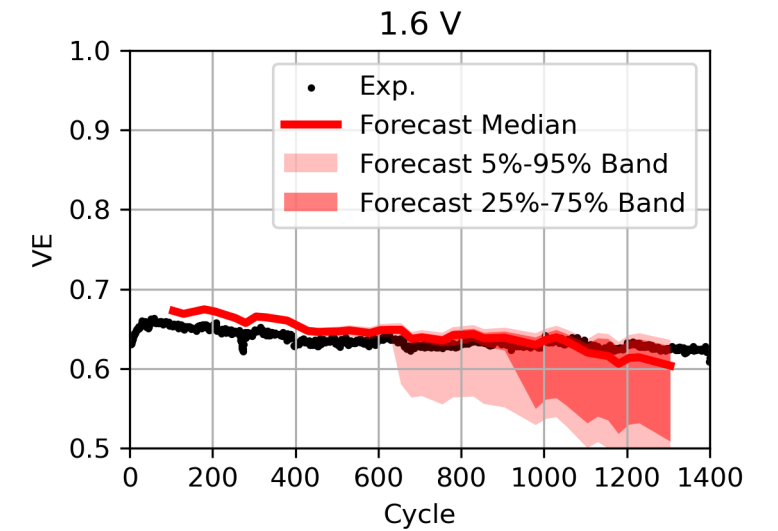
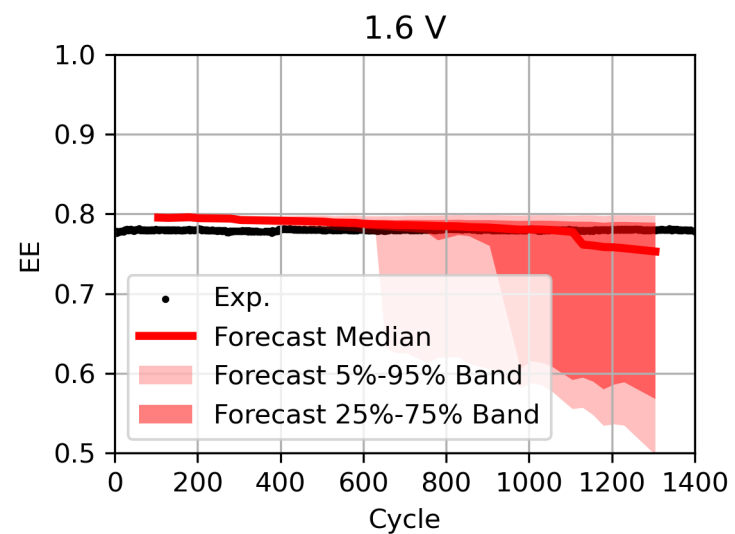
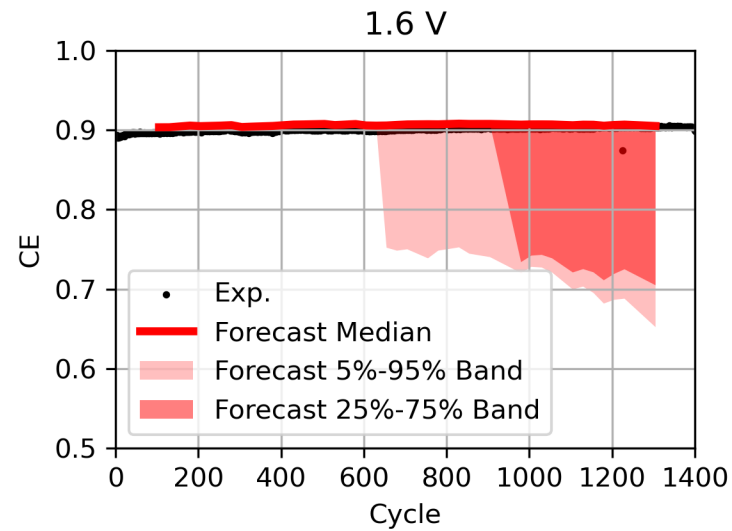
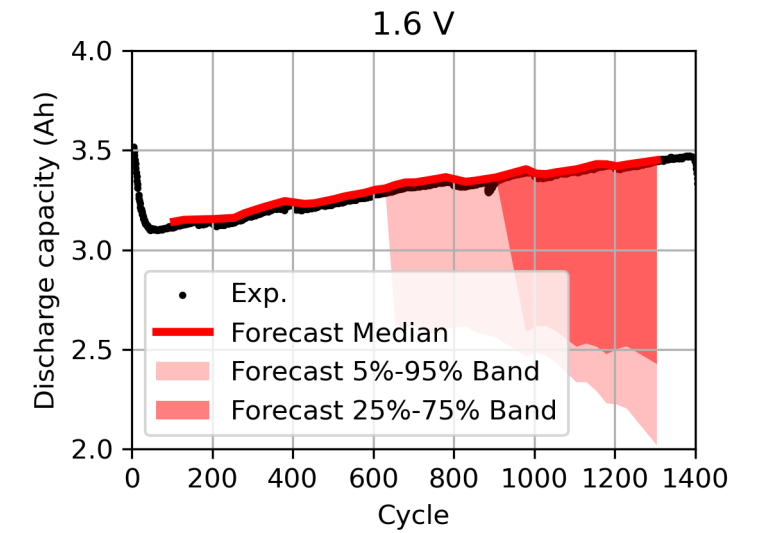
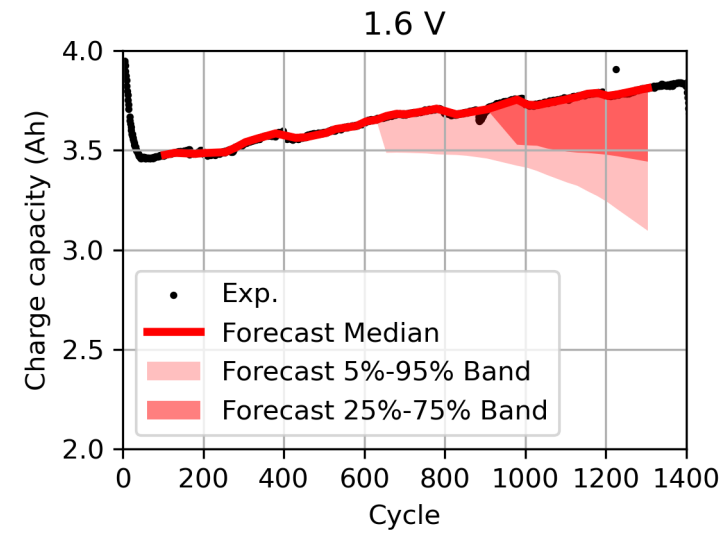


Cycle 1300: Forecast vs. Exp.



# Prognosis Validations

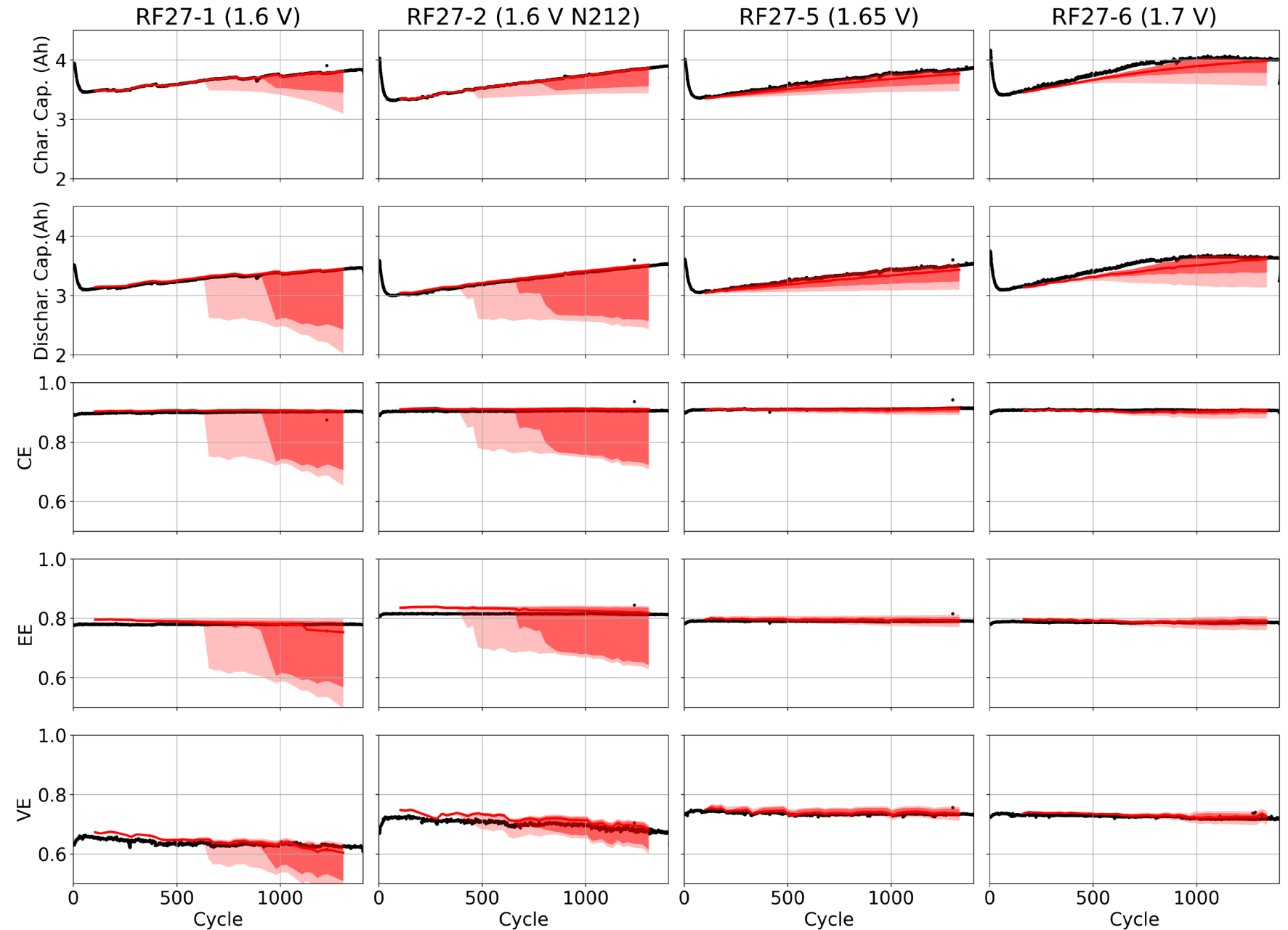
- The forecasted capacities and efficiencies are compared with experimental measurements.



# Prognosis Validations

- The forecasted capacities and efficiencies are compared with experimental measurements for four cases.
- The wider uncertainty bands reflect the risk that the forecasted battery may not be able to support the targeted loading profile.

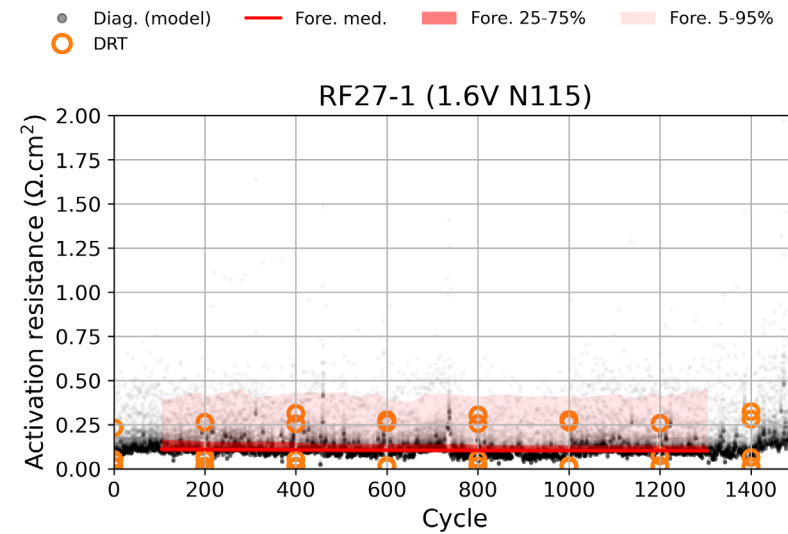
● Exp.    — Forecast Median    ■ Forecast 25%-75% Band    ■ Forecast 5%-95% Band



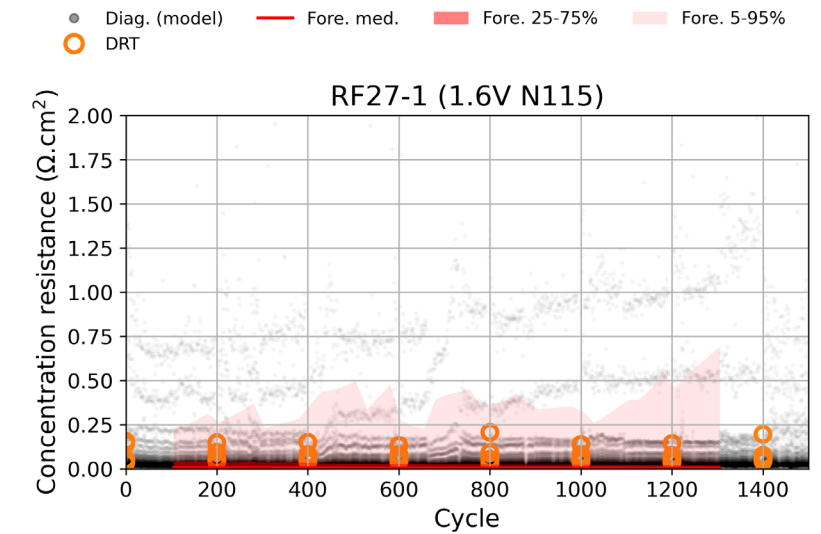
# Prognosis Validations

- The forecasted internal resistance components are compared with results from traditional RPT measurements and analysis.

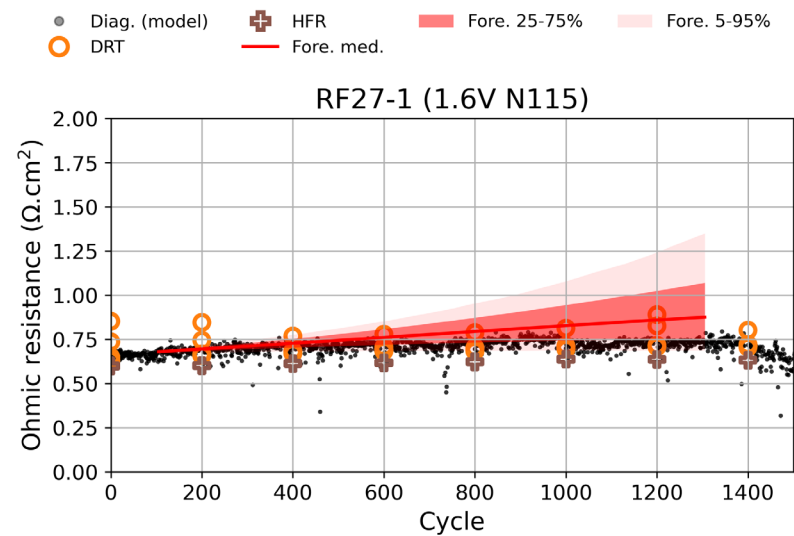
Activation resistance



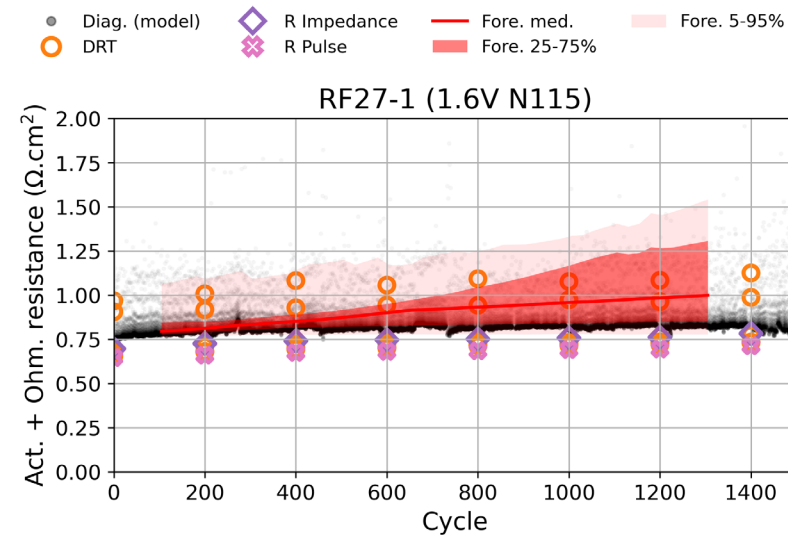
Concentration resistance



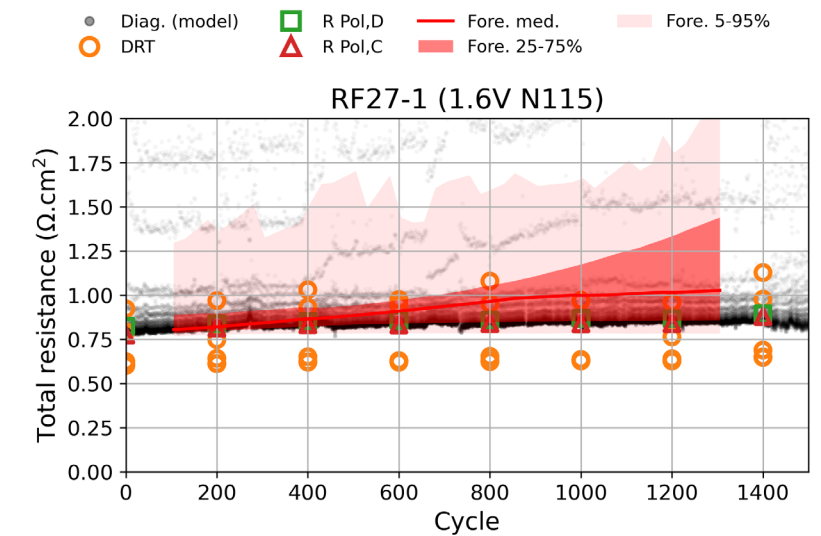
Ohmic resistance



Act. + Ohm. resistance

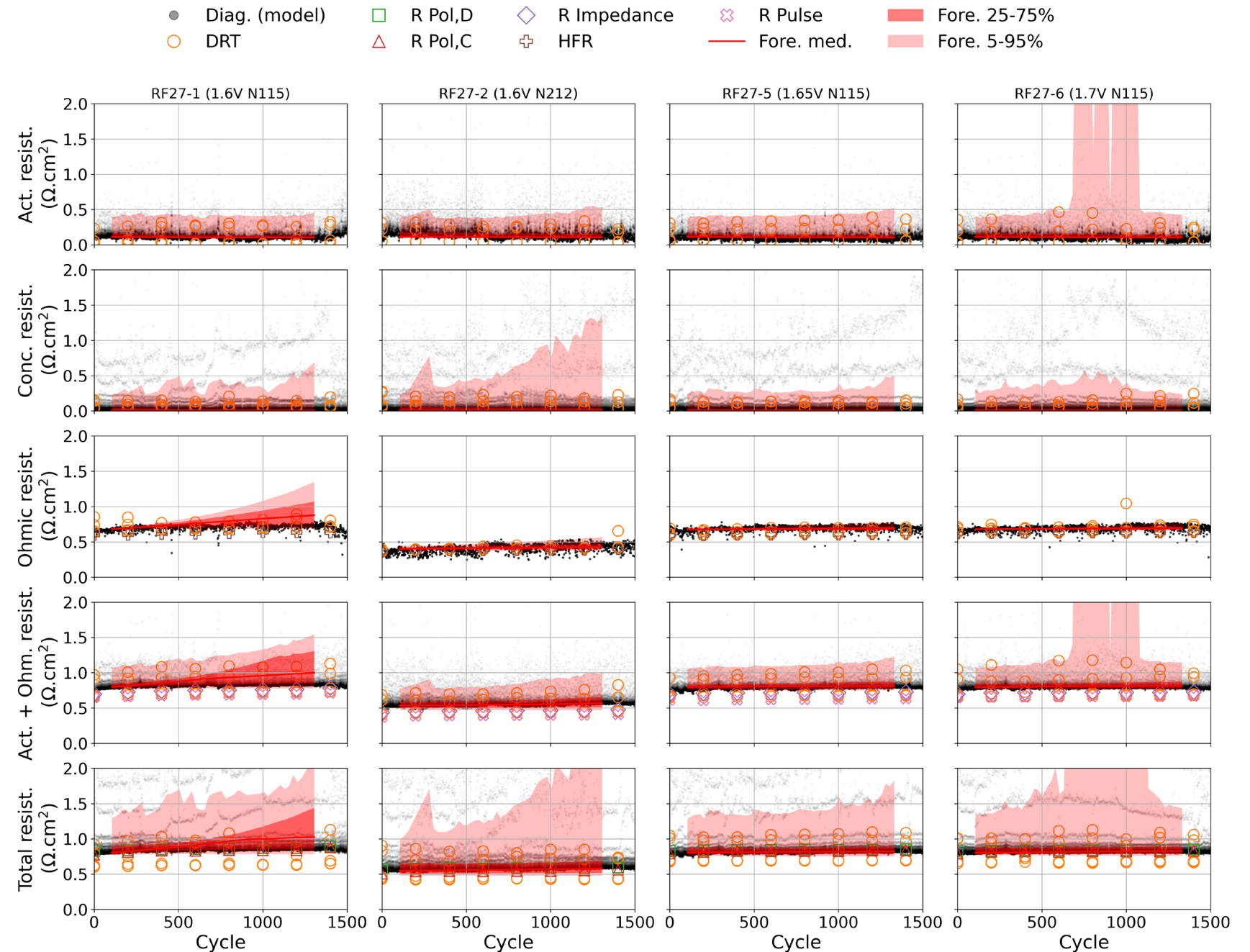


Total resistance



# Prognosis Validations

- The forecasted internal resistance components are compared with results from traditional RPT measurements and analysis across all four cases.
- The 25%–75% uncertainty band captures the traditional RPT measurements well.
- In some cases, the wider 5%–95% uncertainty band reflects the risk that the forecasted battery may not be able to support the targeted loading profile.



# Redox Flow Battery Digital Twin Diagnosis and Prognosis Pipeline

- This research was supported by U.S. Department of Energy (DOE) Office of Electricity's Rapid Operational Validation Initiative (ROVI), and Energy Storage Materials Initiative (ESMI), which is a Laboratory Directed Research and Development Project.

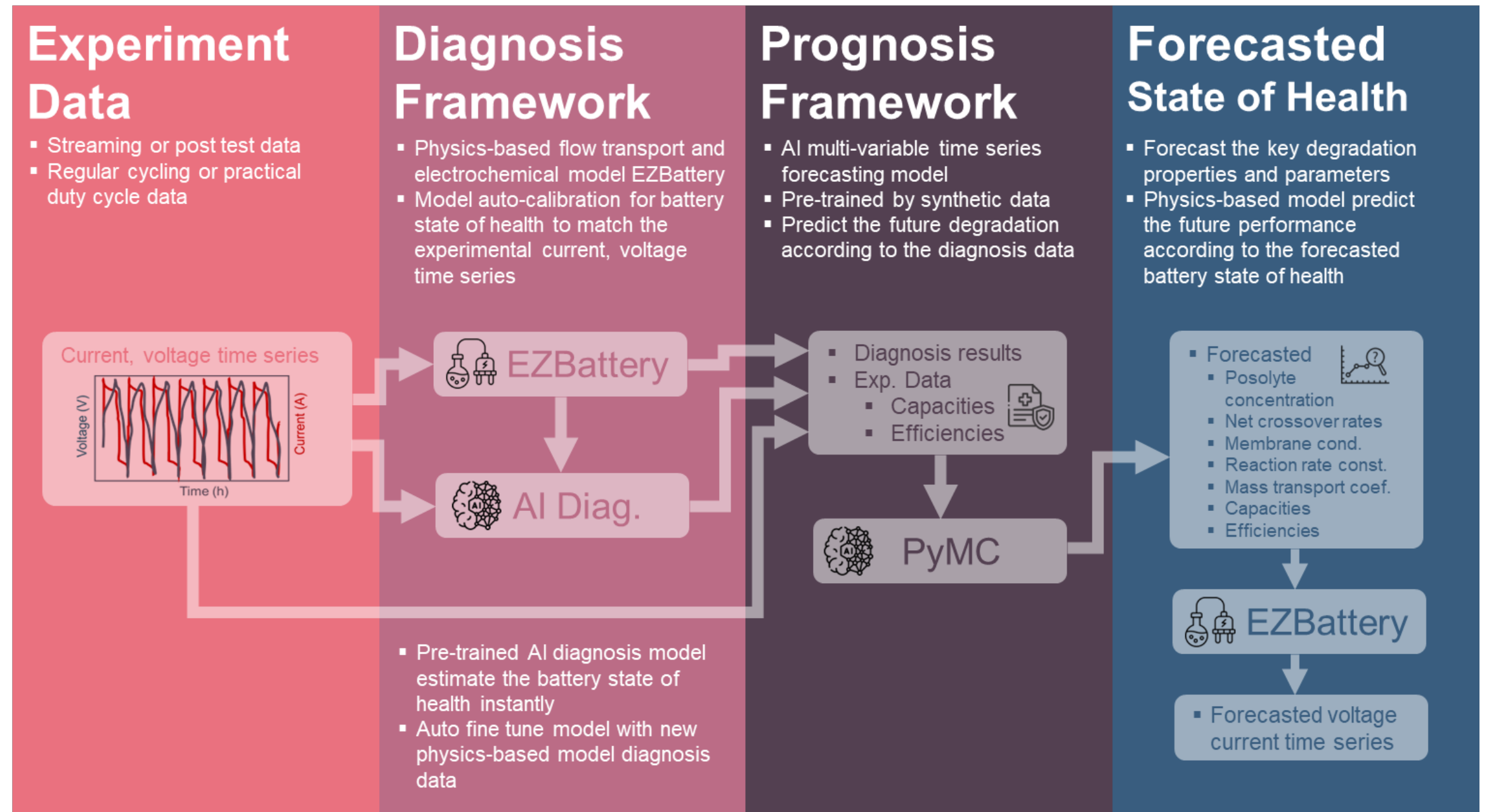
*Journal of Energy Storage*, 2025, 134, Part A, 118134, (DOI <https://doi.org/10.1016/j.est.2025.118134>)

*Journal of Power Sources*, 2025, 635, 23640, (DOI <https://doi.org/10.1016/j.jpowsour.2025.236470>)

*Journal of Power Sources*, 2023, 578, 233210 (DOI <https://doi.org/10.1016/j.jpowsour.2023.233210>)

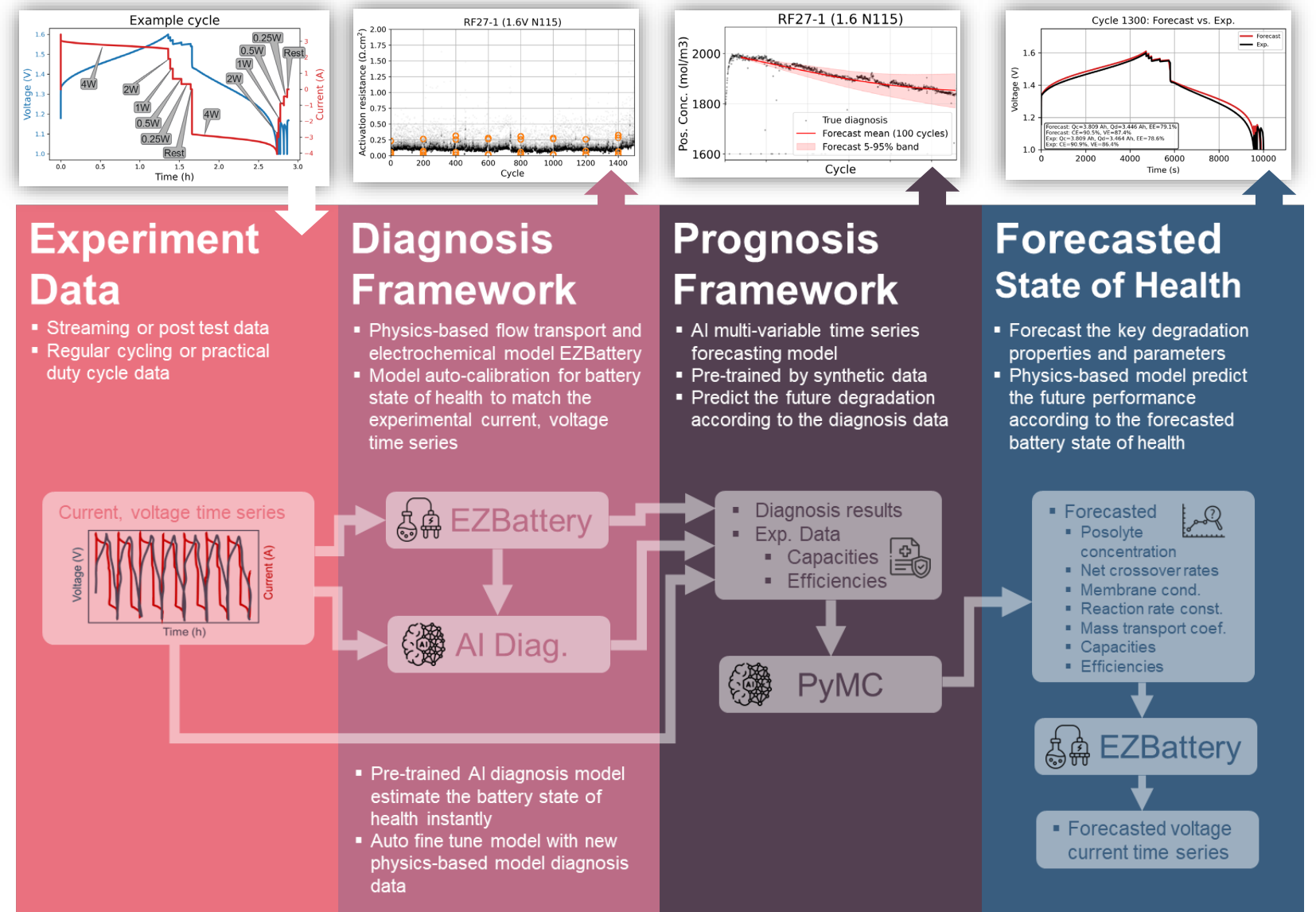
*Journal of Power Sources*, 2021, 506, 230192 (DOI <https://doi.org/10.1016/j.jpowsour.2021.230192>)

*Journal of Power Sources*, 2021, 482, 228817 (DOI <https://doi.org/10.1016/j.jpowsour.2020.228817>)



# Summary

- The redox flow battery digital twin diagnosis and prognosis pipeline has been tested and validated using a lab-scale vanadium redox flow battery with a liquid-bridge configuration.
- The digital twin diagnostic results are in good agreement with traditional RPT measurements and analysis.
- The pipeline is currently being tested on the INVINITY VS3 13 kW system.





**Thank you**

