5.9: Process Twins for Decision-Support and Dynamic Energy/Cost Prediction in Water Reuse Processes

NAWI National Alliance for Water Innovation

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Project Scope and Objectives

Project Scope: Integrating physical and digital twins of water reclamation and reuse systems to enhance operational decision-making.

Key Objectives: 1) Develop an advanced data analytics method (coupled physical digital twin) for water reclamation processes; **2)** Apply advanced analytics methods to optimize the cost and environmental performance of example water reclamation and reuse facilities.

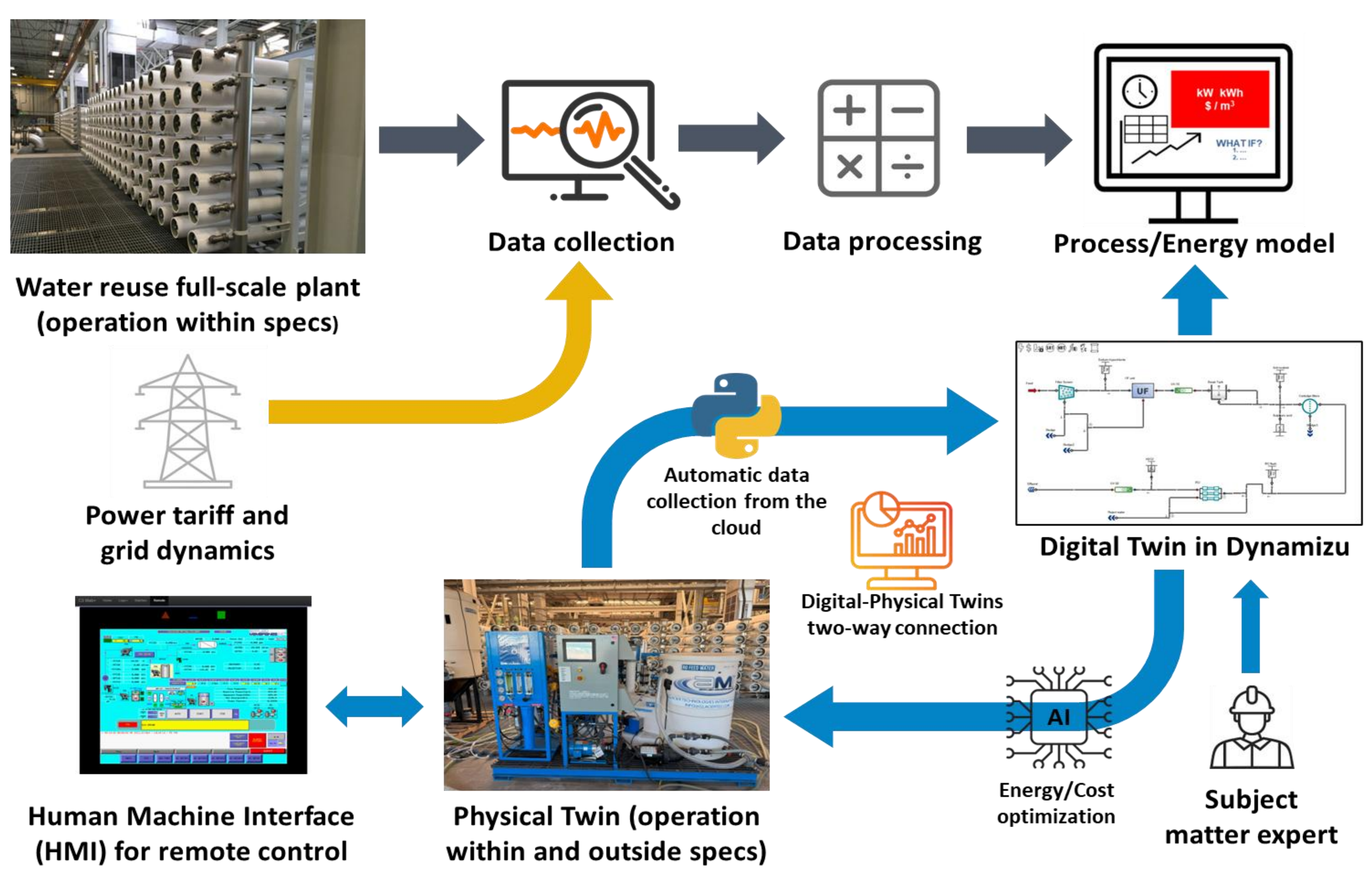
Current Practice and State-of-the-Art

Digital Twins are new to the water sector and their potential is untapped.

Digital-physical twin integration can address:

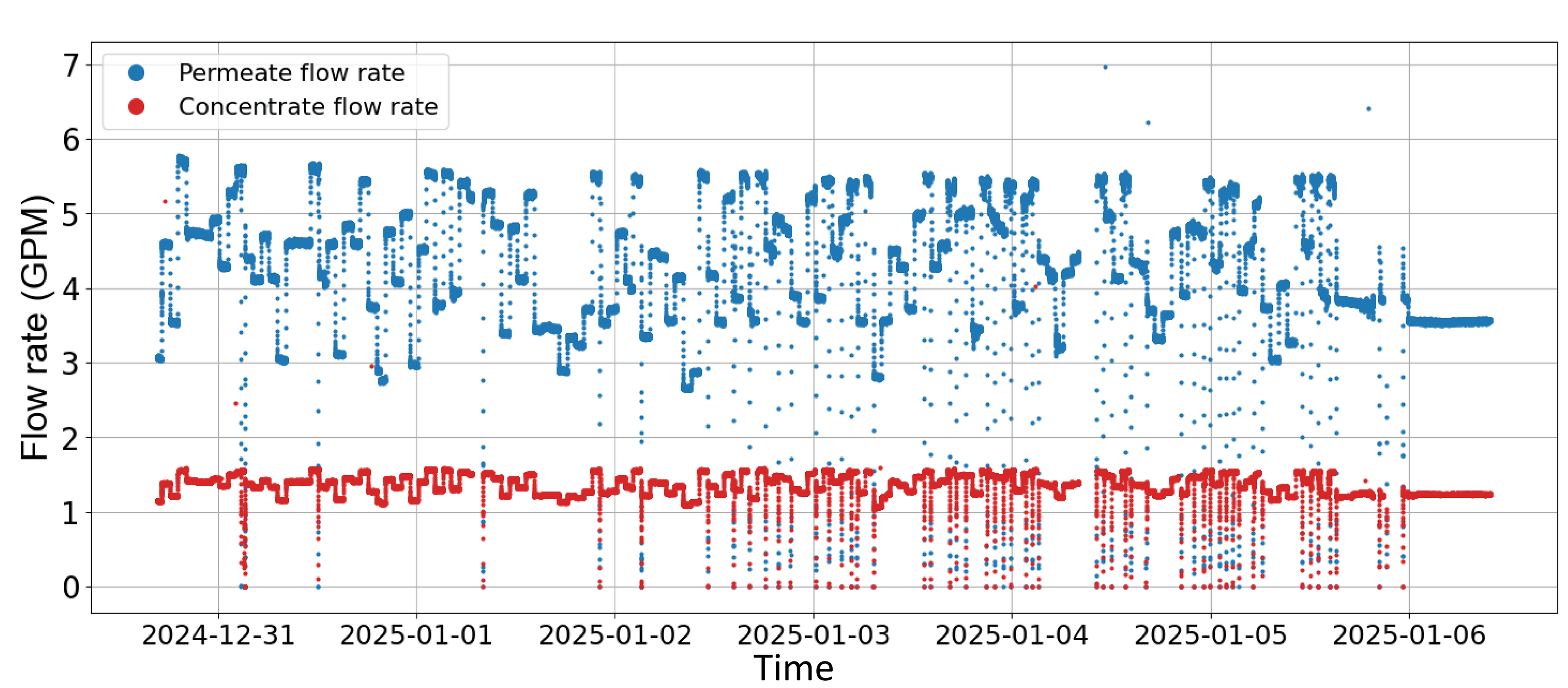
- Data-**sparsity** and **contingency** scenarios;
- **Real-time** operational decision-making and **early warning** for adverse conditions;
- Process performance **optimization** and identification of **improvement** areas.

Approach and Novelty



Sample Results

Physical twin experiment:



Non-stop 7-day pilot operation. The permeate flow set point was changed remotely and automatically every hour, based on the experimental design.

Sparse Machine Learning (ML) for Optimization:

- Physics-based models are computationally intensive
- ML was used to improve system control and efficiency by developing sparse interpretable models
- The model was trained and tested on the 7-day experiment data:

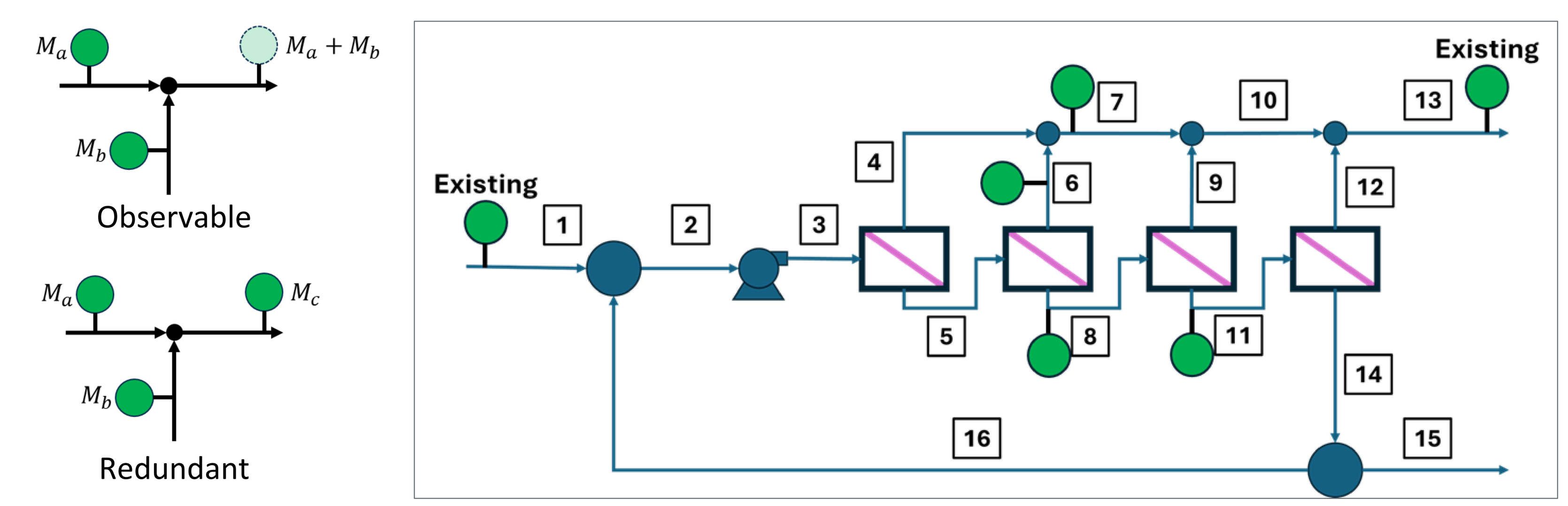
Actual and scaled RMSE results for the LASSO ML model.

Dataset	RMSE Actual	RMSE Scaled (Standardized)
Training	34.27	0.097
Test	24.45	0.072

- Percentage of observations within ±2% error range (Test Data): 95.62%

Soft Sensors and Data QA/QC:

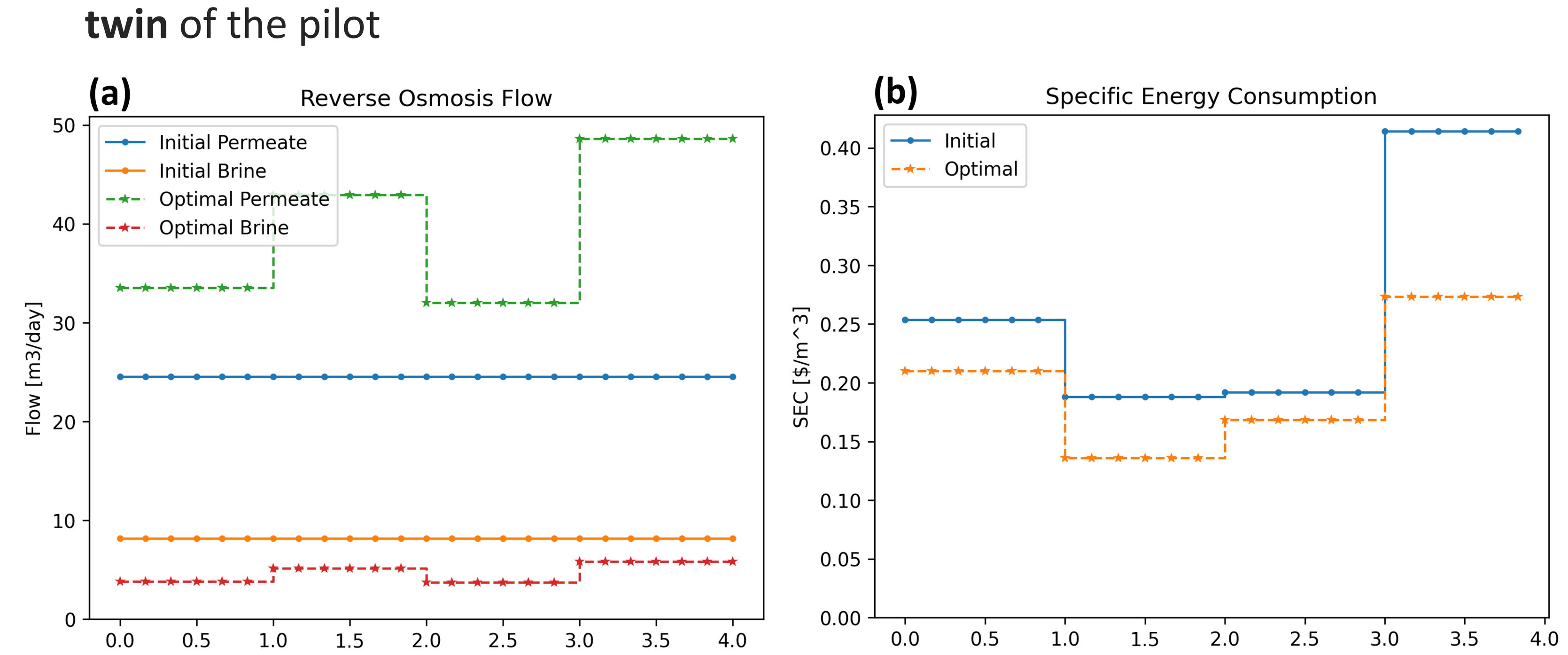
- Established a structural redundancy and observability labeling method for nonlinear pressure systems in a written protocol
- Structural labeling and optimization required before practical observability can be considered



Example of minimum flow sensors needed for full flowrate observability on the pilot

Pilot-scale Cost optimization:

- Developed an **optimization framework** to **vary operating parameters** in response to an **electricity tariff**
- This optimization framework is currently being **tested** on the **dynamic digital twin** of the pilot



*Optimization results for the pilot comparing **(a)** permeate, brine recirculation, and **(b)** specific energy consumption cost.*

- This optimization framework will be translated for use on the full-scale plant at OCWD

NAWI CONNECTIONS

Period of Performance: January 2023 – September 2025

Challenge Area/Topic Area: Topic Area 1 – Process Innovation and Intensification

AOI A-3.1: Predictive algorithms for process control and fault detection

AOI A-3.2: Advanced Process Data Analytics and Modeling

NAWI Leverage:

This project is complementary to NAWI 5.08 since the focus is on membrane-based reuse. In addition to developing code, a dynamic process model simulator (i.e., SUMO by Dynamita and Dynamizu, available to the UCI WEX Center) will be integrated. The project team is also collaborating with the WaterTAP and NAWI 3.23 teams.

KEY FINDINGS AND CONCLUSIONS

Sparse ML model for Optimization: An ML model was developed to improve system control and efficiency

Soft Sensors and Data QA/QC: A structural redundancy and observability labeling method was established

Pilot-Scale Cost Optimization: An optimization framework was developed for the pilot-scale system and will be translated to the full-scale system.

Analysis of knowledge transfer: Interviews with industrial stakeholders are ongoing, to understand barriers to technology adoption

IMPACTS:

- The project provides crucial information on the approaches and challenges associated with the **implementation of a full-scale Digital Twin** system in the water industry.
- The outcomes will provide critical information regarding the **dynamic energy and cost optimization** of water reuse systems, as well as addressing the potential **system anomalies**.
- This is the **first effort** to implement a full-scale Digital Twin system with all the required elements, and **two-way communication** with the physical twin in the water sector (including the **dynamic energy overlay**).

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ACKNOWLEDGEMENTS

The research team thanks Guy Gutterman, Carol Valladao, Peter Fiske, and the whole NAWI team for their invaluable help during the contracting phase. Special thanks to the treatment plant personnel who support this project (Megan Plumlee, Han Gu, Don Supernaw, Chris Wilson, Germano Salazar-Benites, and Nikos Melitas).

This material is based upon work supported by the National Alliance for Water Innovation (NAWI), funded by the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy (EERE), Industrial Efficiency and Decarbonization Office under Funding Opportunity Announcement DE-FOA-0001905.

This material is based upon work supported by the National Alliance for Water Innovation (NAWI), funded by the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy (EERE), Industrial Efficiency and Decarbonization Office, under Funding Opportunity Announcement DE-FOA-0001905.

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Brown & Caldwell
Glacier Technology Inc

UCI WEX Center — Research at the Water-Energy Nexus

Oak Ridge National Laboratory