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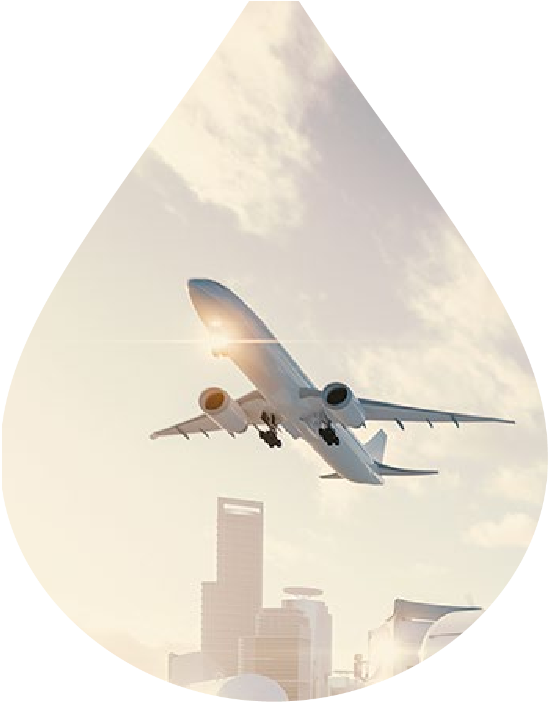
Accelerating the new hydrogen economy in the Midlands

SOFC System Longevity: Advanced Modelling, Optimisation, and Machine Learning Predictions



Clyde-Theodore Batista
28th April 2025

Aston University

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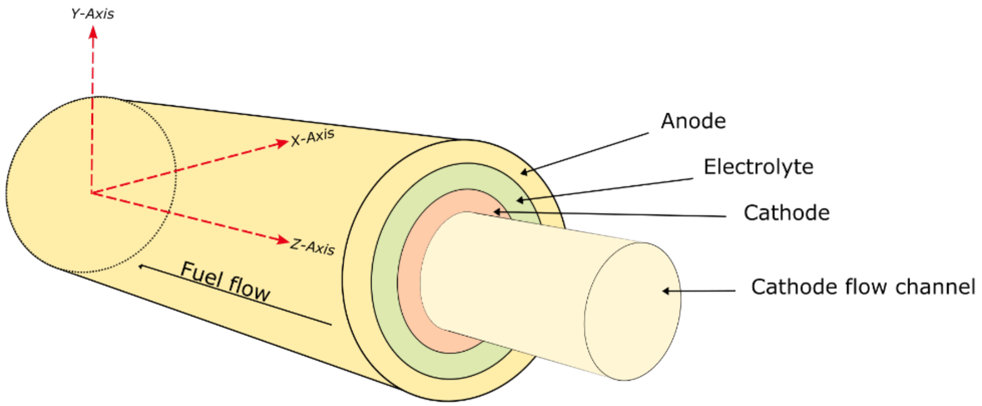
Introduction: What are SOFCs?

- Solid Oxide Fuel Cells (SOFCs) convert chemical energy directly into electrical energy through electrochemical reactions.
- Offer high electrical efficiencies (typically range from 40% to 60%), reaching up to 80% in CHP applications.
- Primarily utilise hydrogen as fuel but can also operate on various hydrogen carriers with appropriate reforming and impurity removal strategies.
- Commonly applied in off-grid power generation, Combined Heat and Power (CHP) systems, and emergency back-up power.



RESEARCH MOTIVATION

Challenges:

- Durability issues: thermal mismatch, multifaceted degradation, local instabilities.
- Lack of large, high-quality experimental datasets.
- Difficulty replicating real-world degradation in system models.

Motivation:

- Commercialisation hindered by durability and lifetime uncertainties.
- End-of-life and second-life pathways poorly defined.
- Insufficient data limits accurate lifetime prediction and maintenance planning.

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RESEARCH AIMS

- **Optimise system configurations** (multi-staging, AOGR) to enhance fuel utilisation and **extend system lifetime**.
- Build and validate a machine learning framework (**BiLSTM**) for predicting voltage degradation and Remaining Useful Life (RUL).
- Commission experimental equipment and establish baseline performance characteristics of SOFCs.
- Evaluate initial SOFC durability to inform and define future experimental testing plan.
- Propose an **integrated methodology** combining experimental, simulation, and machine learning approaches for future SOFC lifetime prediction.

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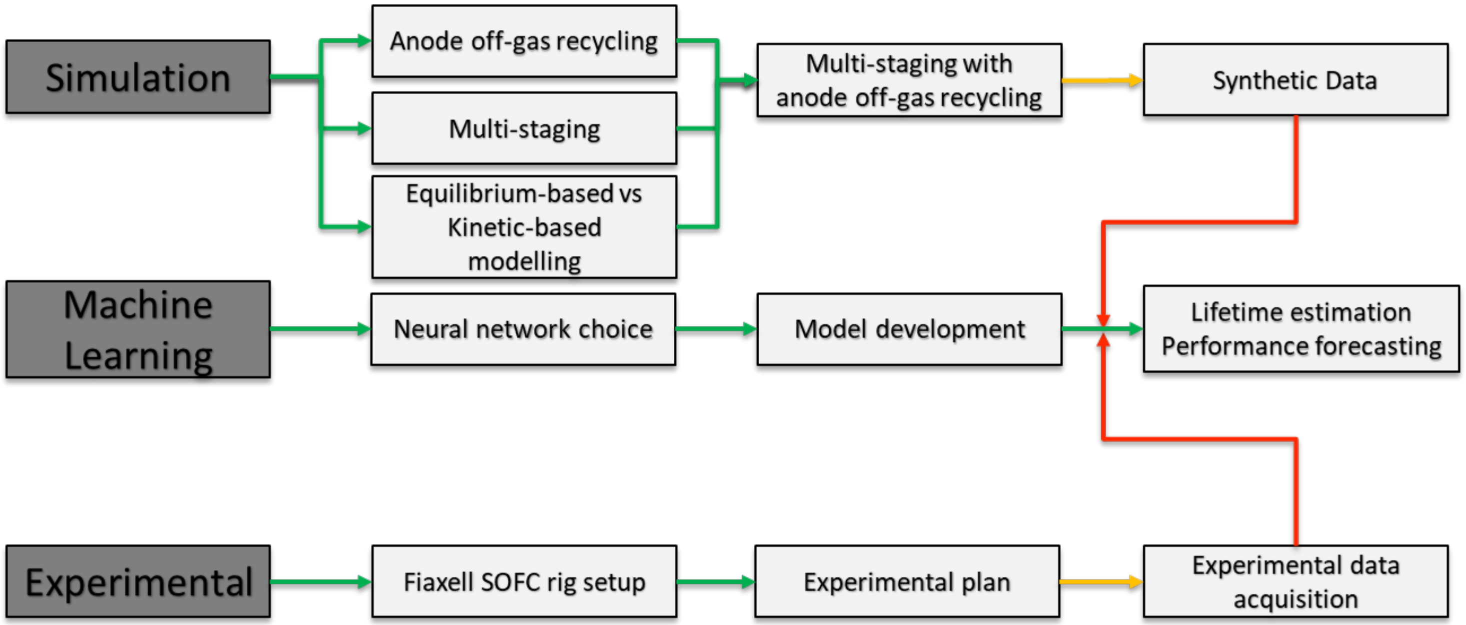
RESEARCH OVERVIEW



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Aspen Simulation: Base Model

- Electrochemical parameters were calculated using **semi-empirical** relations from Zhang et al.
- The base design is based on the Siemens-Westinghouse SOFC platform.
- All subsequent system configurations were developed by adapting this model.

Variable/Parameter	W. Zhang et al., 2005	W. Doherty et al., 2010	T. R. Tanim, 2012	This work	% Deviation
Voltage, (V)	0.70	0.68	0.69	**0.69**	**0**
Current density, (mA/cm²)	178.0	182.9	182.0	**180.7**	**-0.15**
Pre-reforming temperature, (ºC)	536.0	535.1	535.0	535.1	-0.05
Cathode inlet temperature, (ºC)	821.3	823.7	826.0	826.0	0.28
Stack exhaust temperature, (ºC)	834.0	833.7	836.0	793.9	-4.87
Anode outlet composition					
H_2O	50.9%	50.9%	50.9%	50.9%	0.00
CO_2	24.9%	24.9%	24.9%	24.9%	0.00
H_2	11.6%	11.6%	11.6%	11.6%	0.00
CO	7.4%	7.4%	7.4%	7.4%	0.00
N_2	5.1%	5.1%	5.1%	5.1%	0.00
Stack exhaust composition					
N_2	77.3%	77.3%	77.2%	77.3%	0.04
O_2	15.9%	15.9%	15.7%	15.9%	0.42
H_2O	4.5%	4.5%	4.7%	4.5%	-1.46
CO_2	2.3%	2.3%	2.4%	2.3%	-1.43
Gross electrical efficiency (LHV), (%)	52.0%	51.3%	51.7%	**52.0%**	**0.65**

Zhang, W., Chan, S.H., and Li, J., 2005. Simulation of a tubular solid oxide fuel cell stack using AspenPlus™ unit operation models. Energy Conversion and Management, 46(2), pp.181–196.
Doherty, W., Reynolds, A., and Kennedy, D., 2010. Computer simulation of a biomass gasification-solid oxide fuel cell power system using Aspen Plus. Energy, 35(12), pp.4545–4555.
Tanim, T.R., 2012. Modelling of a 5kWe Solid Oxide Fuel Cell Based Auxiliary Power Unit Operating on JP-8 Fuel.

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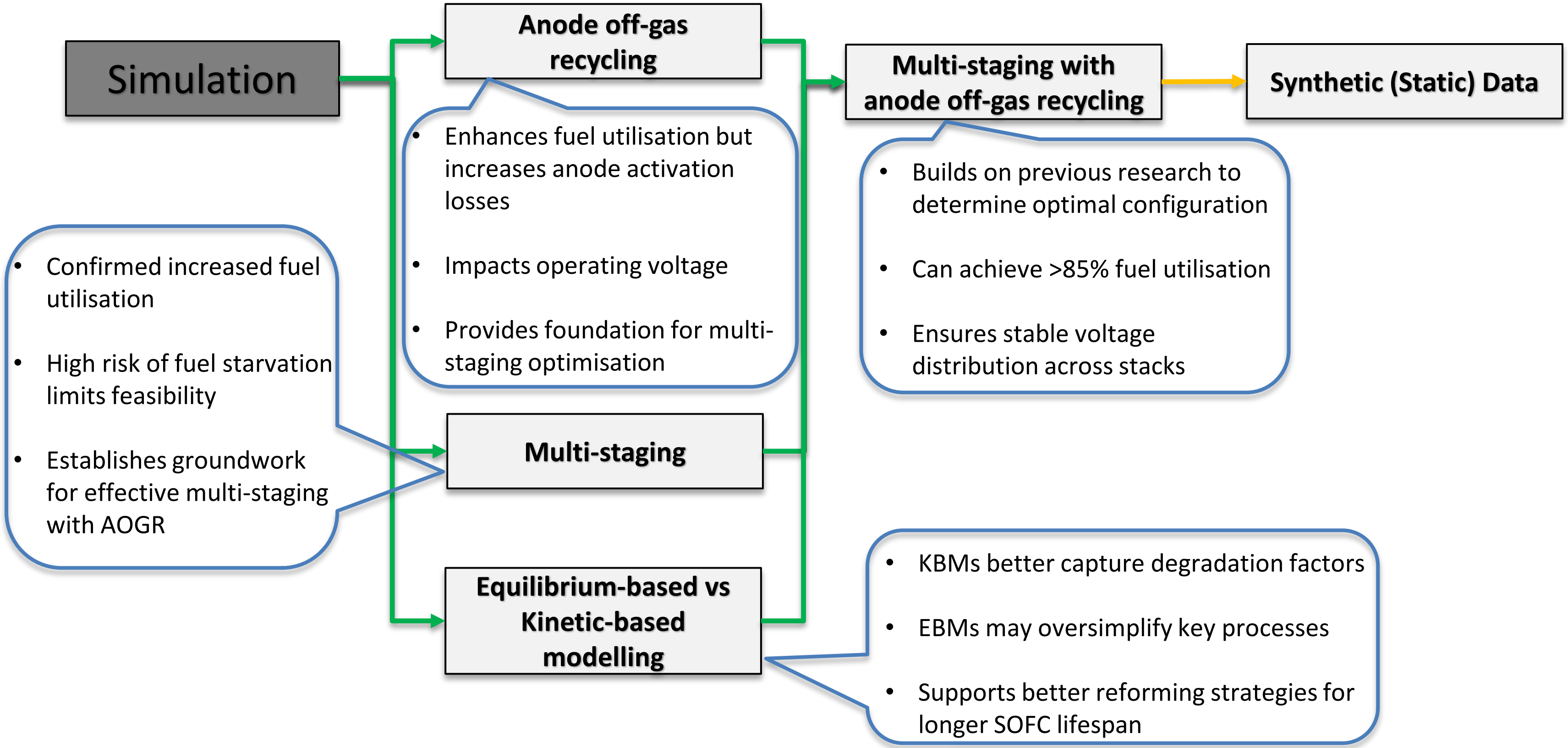
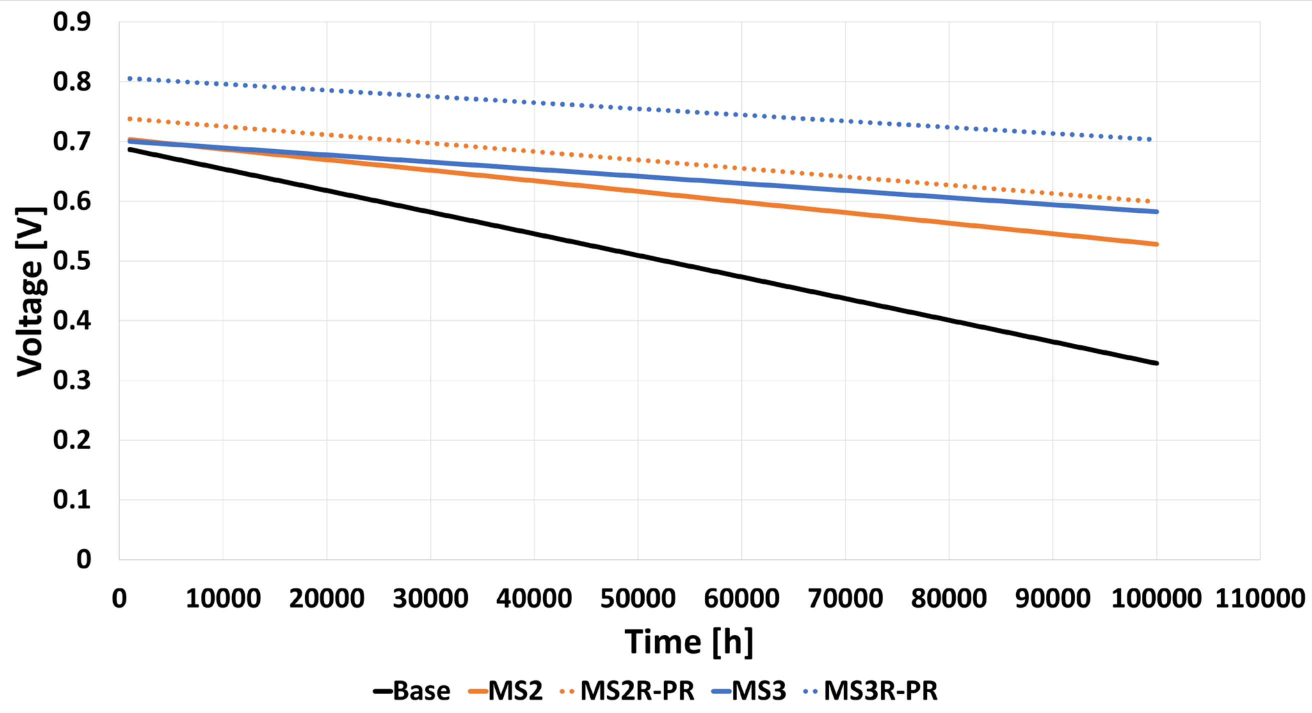
System Configuration: Optimisation

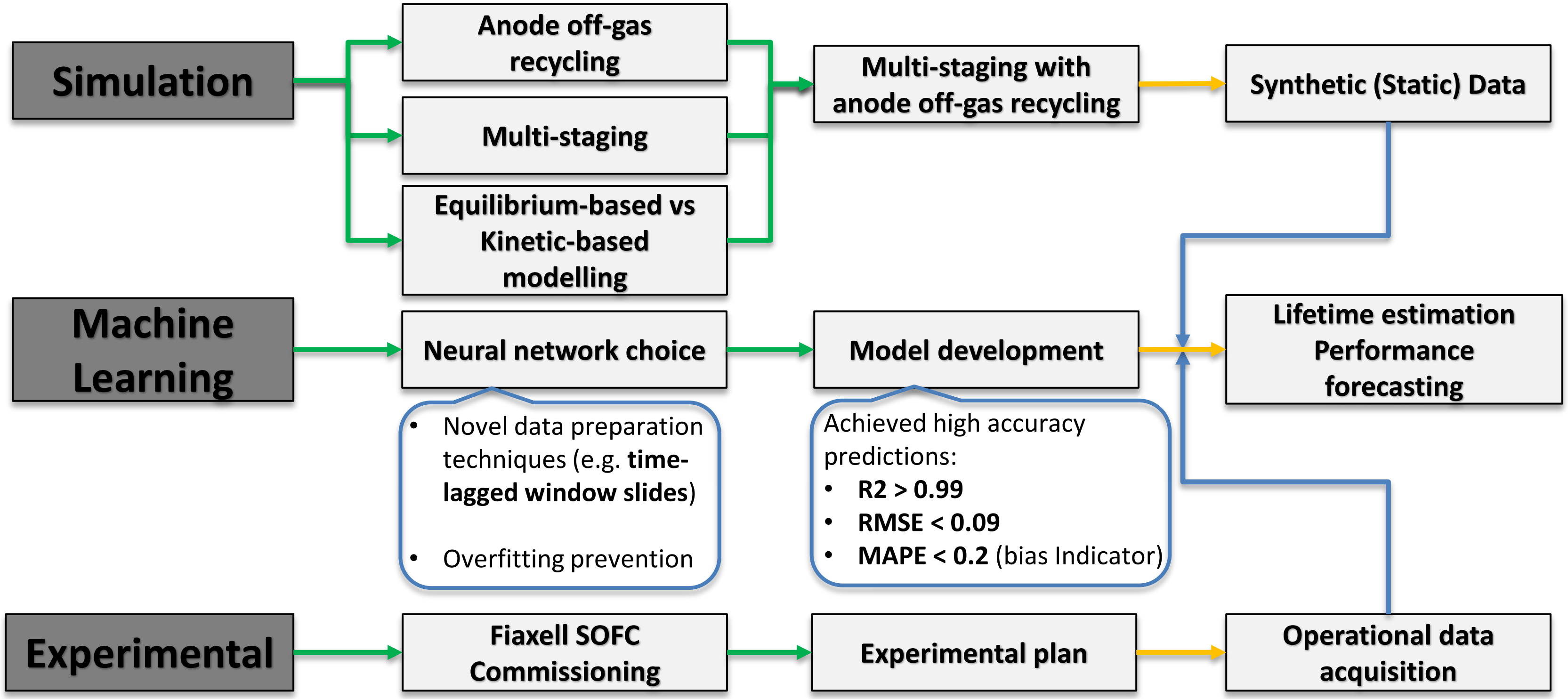


System Configuration: ASR RUL

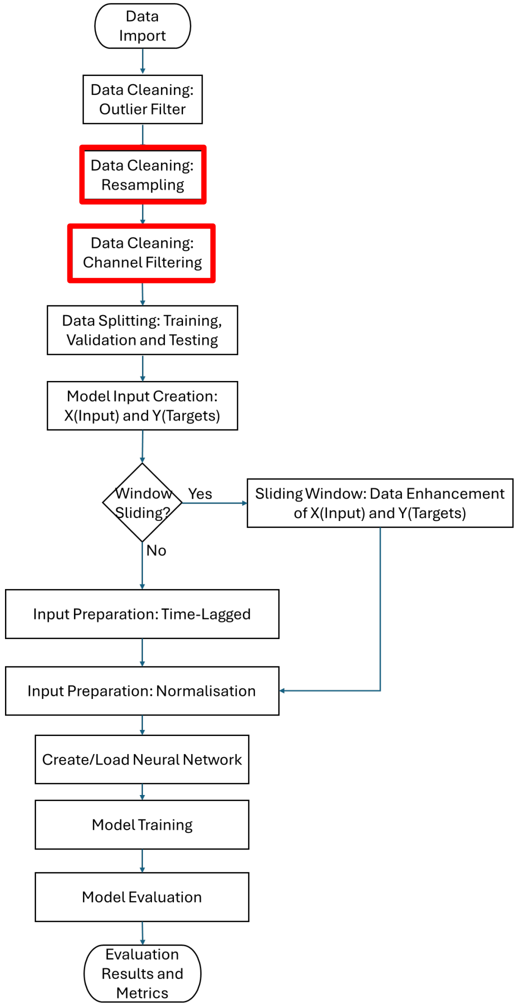
		Voltage	Current Density	Efficiency	Fuel Utilisation
Base	System	0.69	180.7	52%	0.85
MS2	Stack 1	0.77	81.3	24%	0.32
	Stack 2	0.71	88.5	36%	0.49
	System	1.47	84.9	52%	0.65
MS2R-PR	Stack 1	0.77	94.9	36%	0.40
	Stack 2	0.74	70.4	43%	0.57
	System	1.51	82.6	62%	0.85
MS3	Stack 1	0.79	52.8	18%	0.32
	Stack 2	0.77	54.1	26%	0.32
	Stack 3	0.70	59.4	39%	0.46
	System	2.26	55.4	54%	0.75
MS3R-PR	Stack 1	0.82	50.8	22%	0.32
	Stack 2	0.84	49.6	33%	0.32
	Stack 3	0.81	51.6	48%	0.51
	System	2.47	50.7	67%	0.85

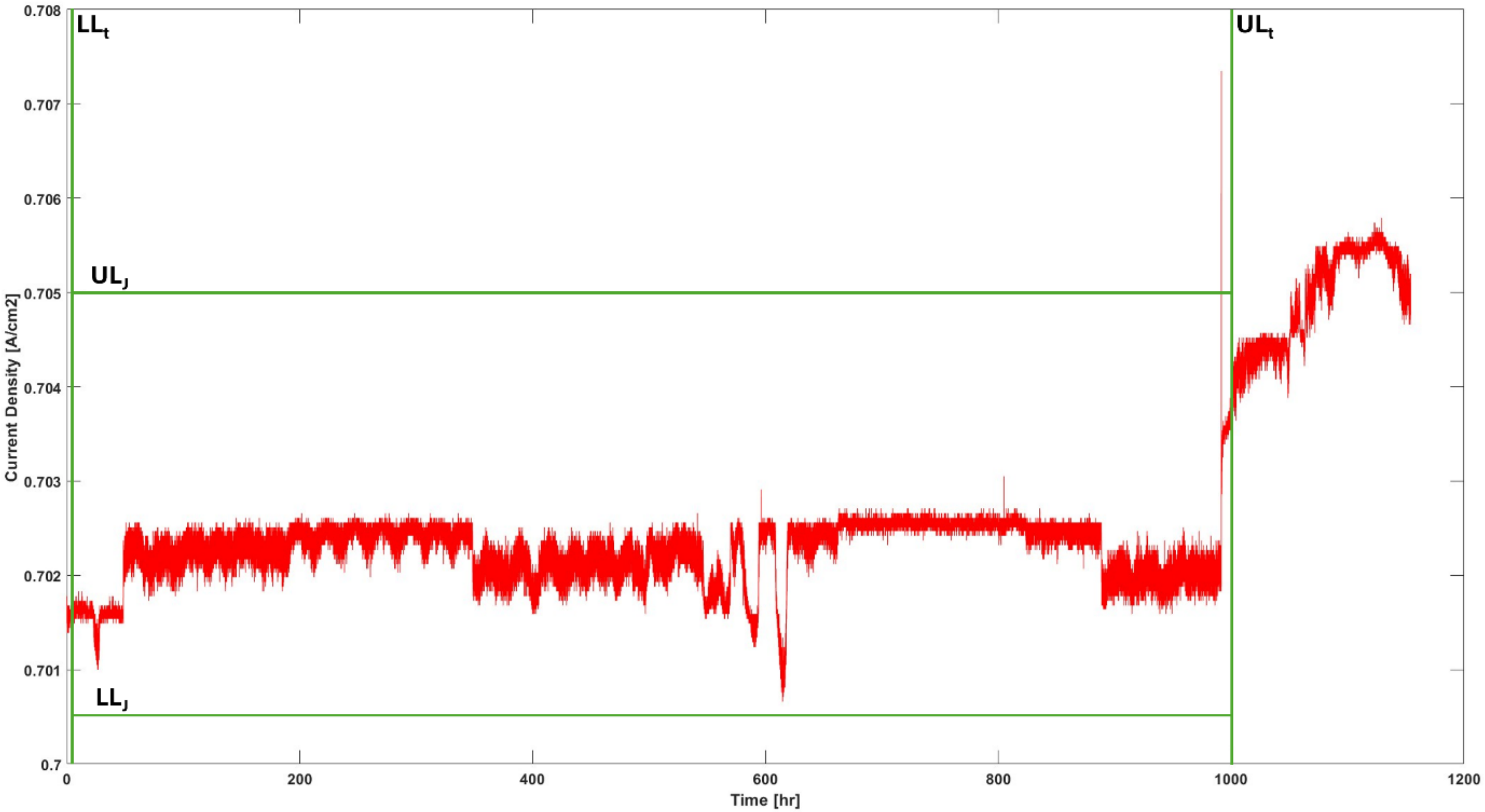


AI-Based Machine Learning



ML: Data Pre-Processing





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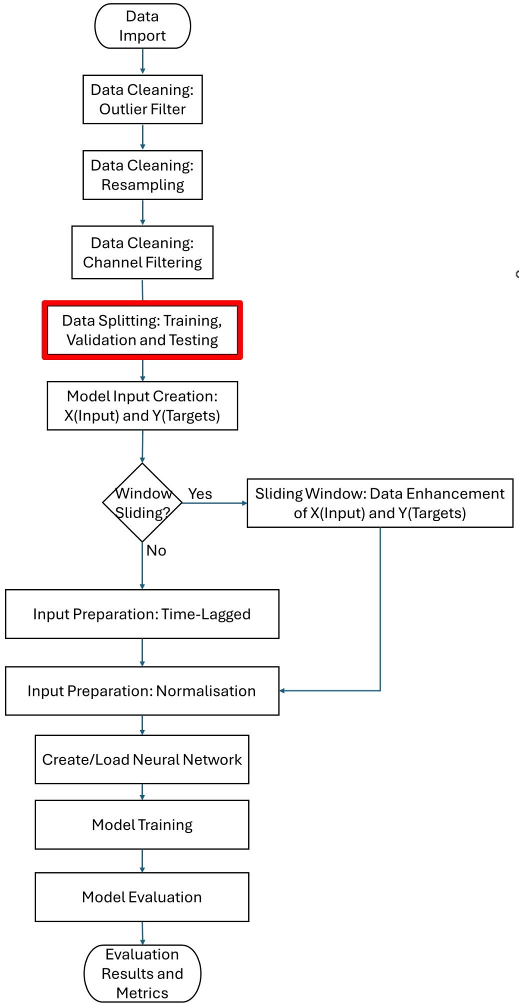

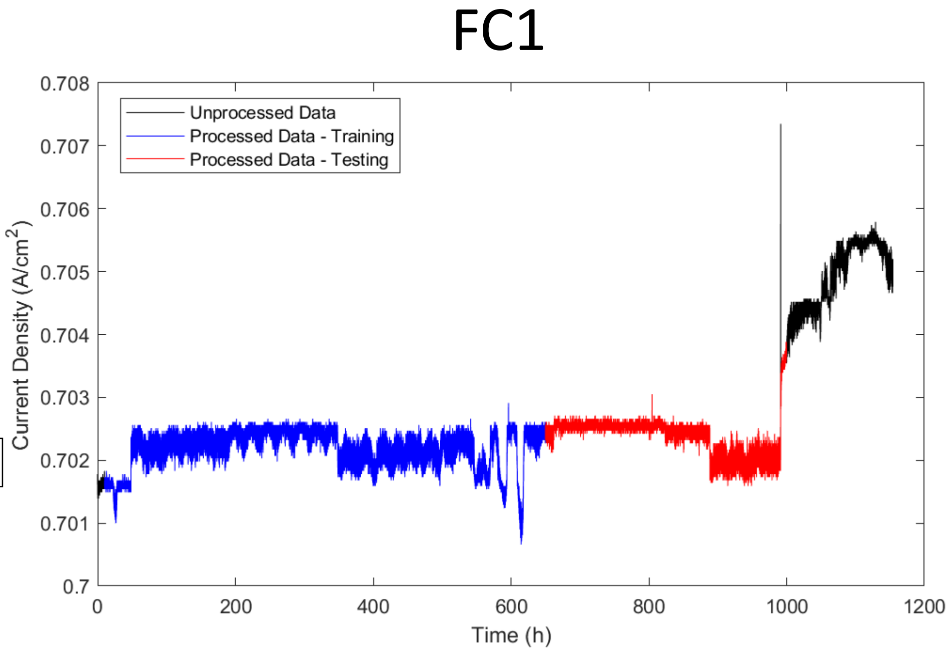

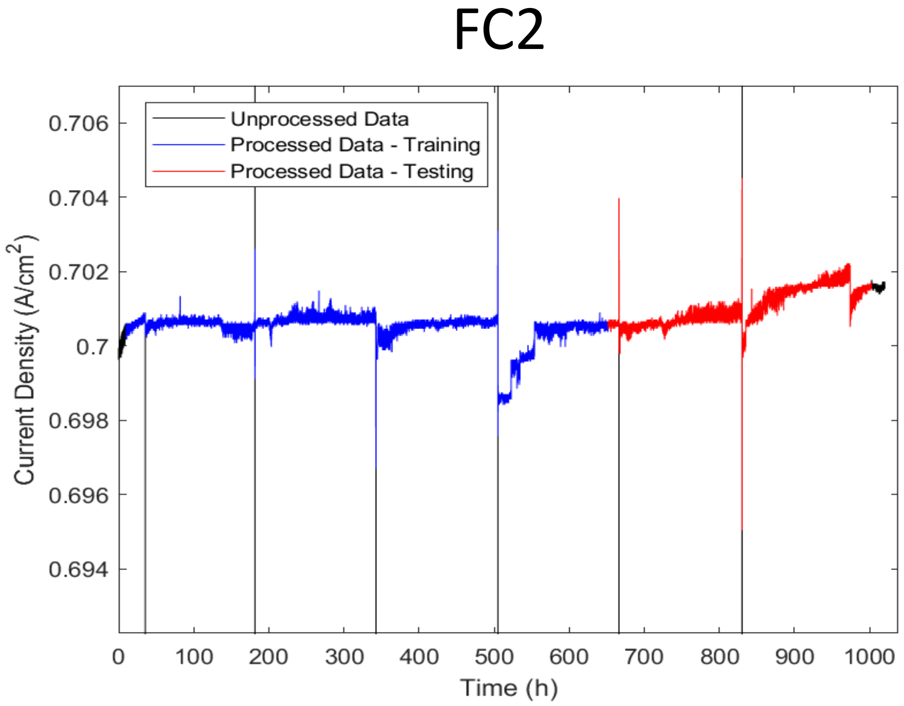

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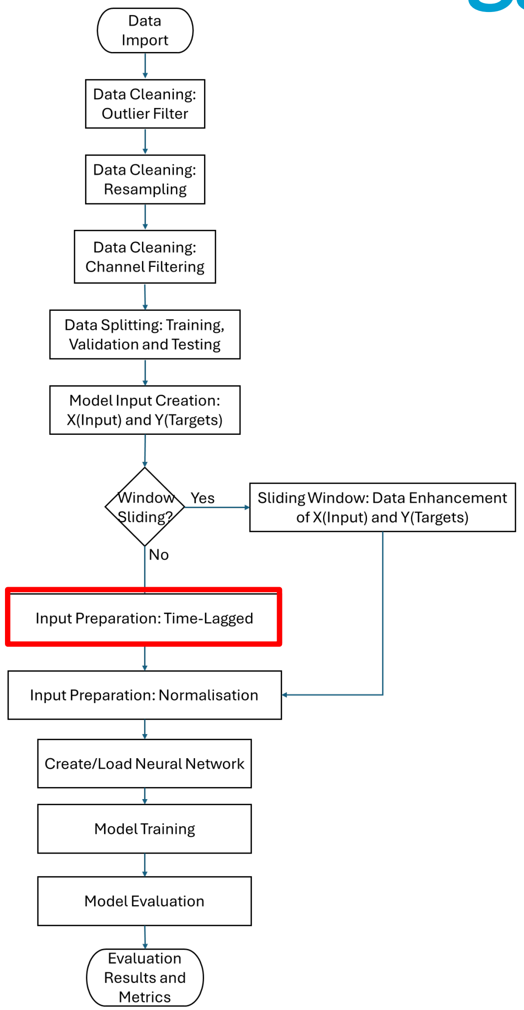
ML: Time-Lagged Inputs



Time (h)	Current (A)	H_2, T_{in} (°C)	Voltage (V)
0	70.164	25.93	3.317
0.000156	70.164	25.945	3.317
0.000321	70.164	25.943	3.316
0.000475	70.164	25.945	3.316
0.000624	70.164	25.939	3.316
0.000794	70.164	25.956	3.317
0.000951	70.164	25.951	3.317
0.001103	70.164	25.939	3.317
0.001258	70.164	25.956	3.317
0.001409	70.164	25.951	3.316

Predictors (X)

Time (h)	Current (A)	H_2, T_{in} (°C)	Voltage (V)
0	70.164	25.93	3.317
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Target (Y)

Time (h)	Current (A)	H_2, T_{in} (°C)	Voltage (V)
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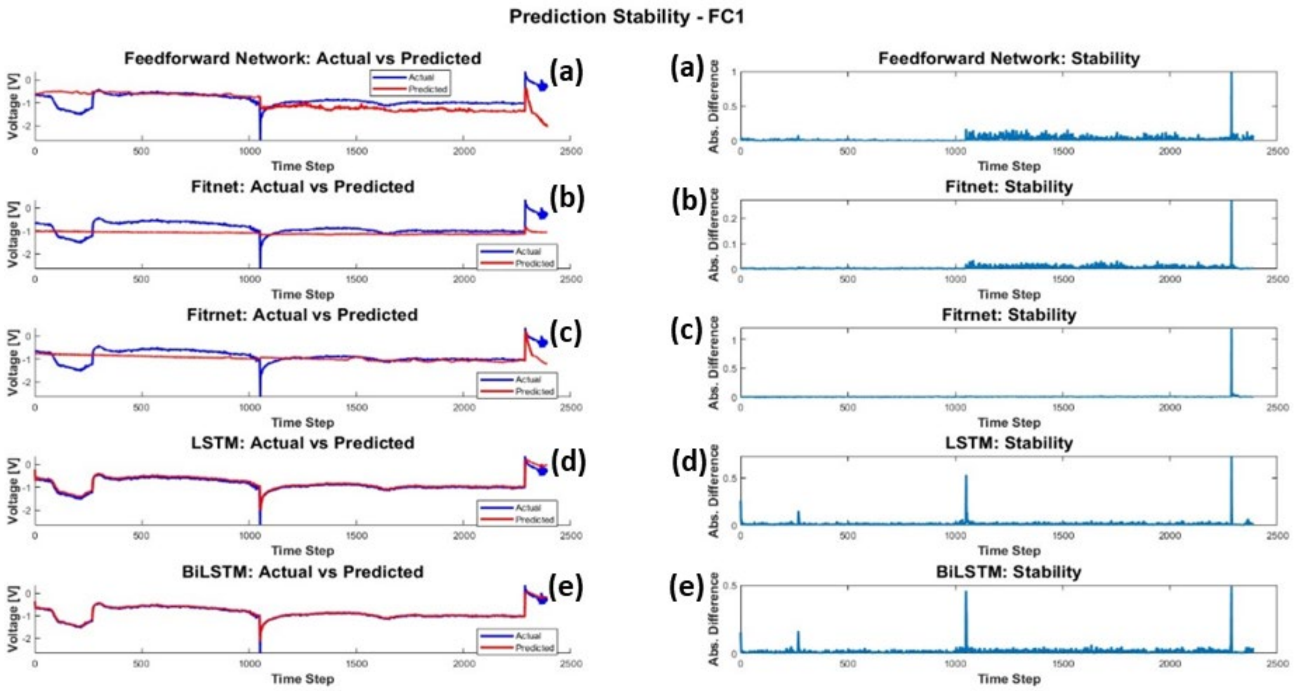
ML: Neural Network Selection



METRIC	Feedforward	FitNet	FitrNet	LSTM	BiLSTM
FC1					
R2	-1.293	-0.564	0.022	0.977	0.991
RMSE	0.419	0.346	0.274	0.090	0.053
MSE	0.176	0.120	0.075	0.009	0.004
MAE	0.291	0.287	0.197	0.064	0.033
MAPE	106.155	110.939	58.237	0.125	0.065
FC2					
R2	-0.990	-2.016	-1.766	0.991	0.988
RMSE	0.828	1.019	0.976	0.062	0.066
MSE	0.685	1.038	0.952	0.014	0.018
MAE	0.696	0.859	0.826	0.049	0.052
MAPE	34.147	49.517	41.990	0.413	0.359

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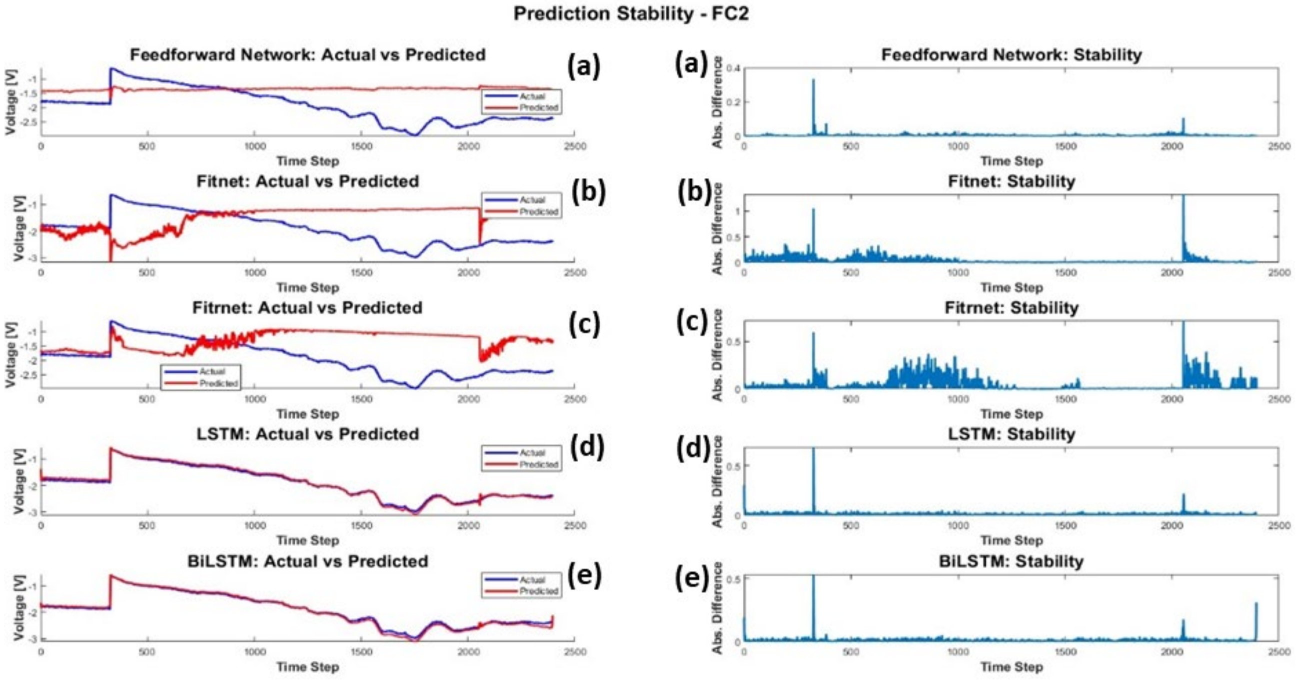
ML: Neural Network Selection



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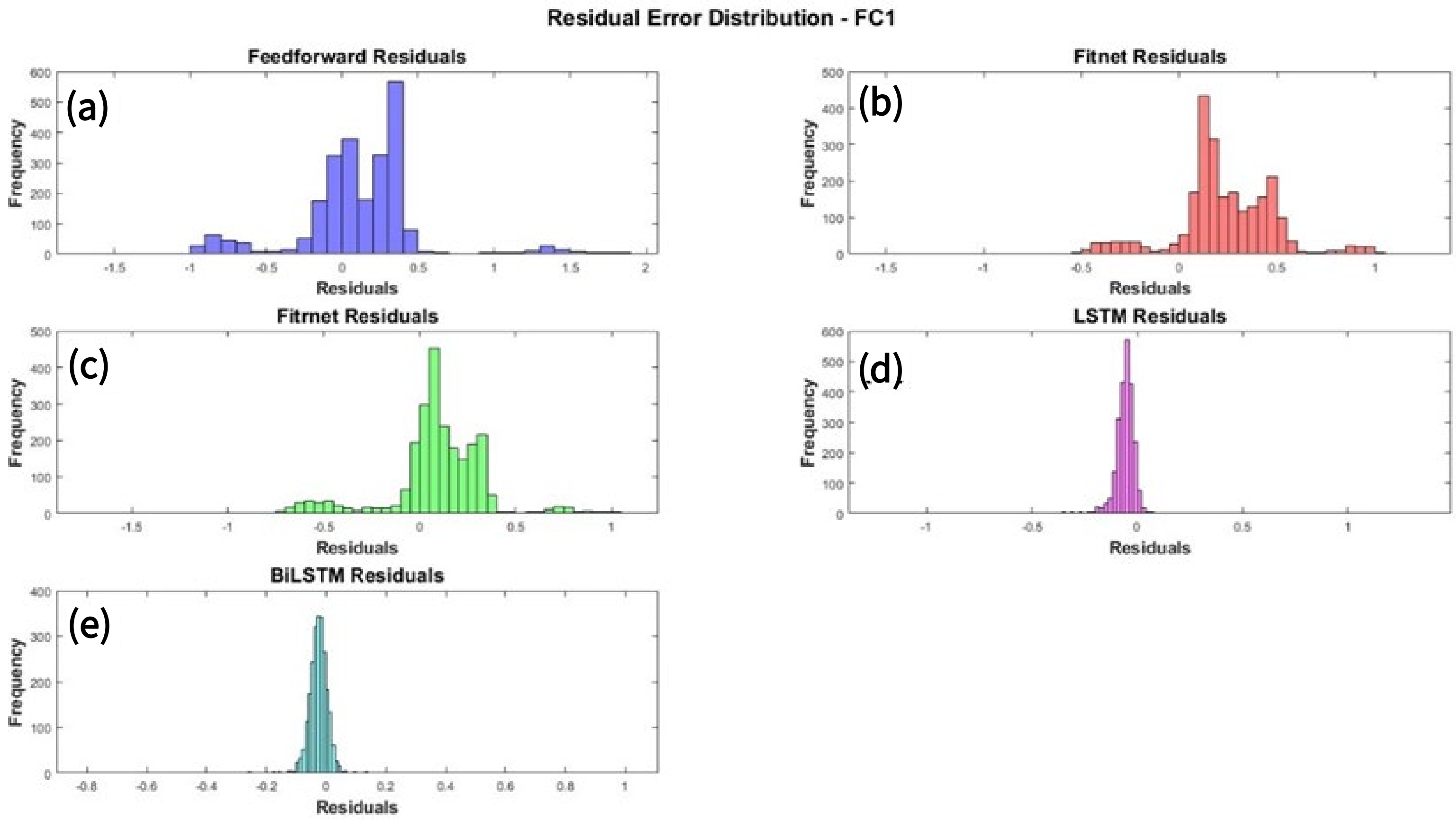
ML: Model Results and Validation



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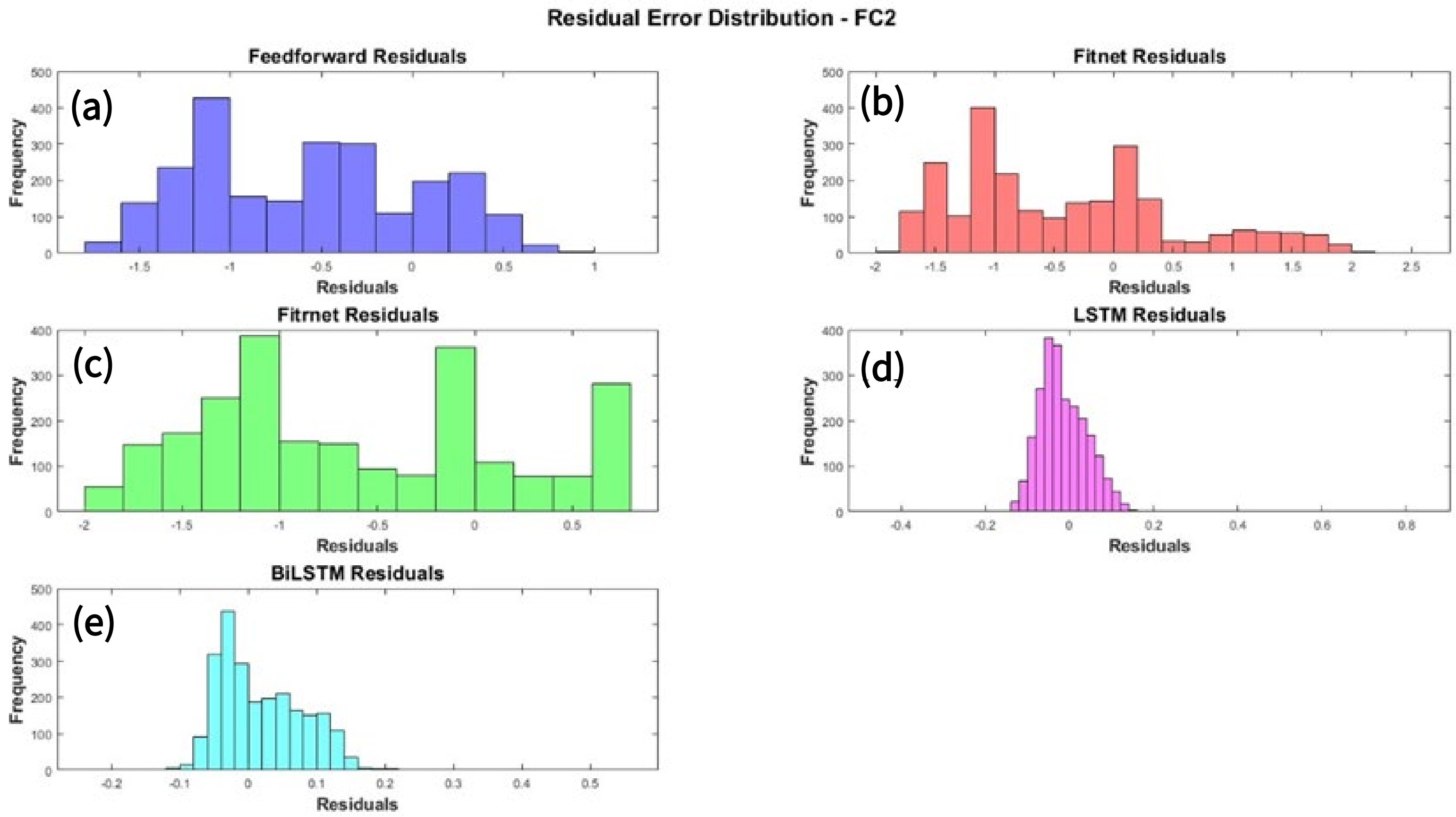

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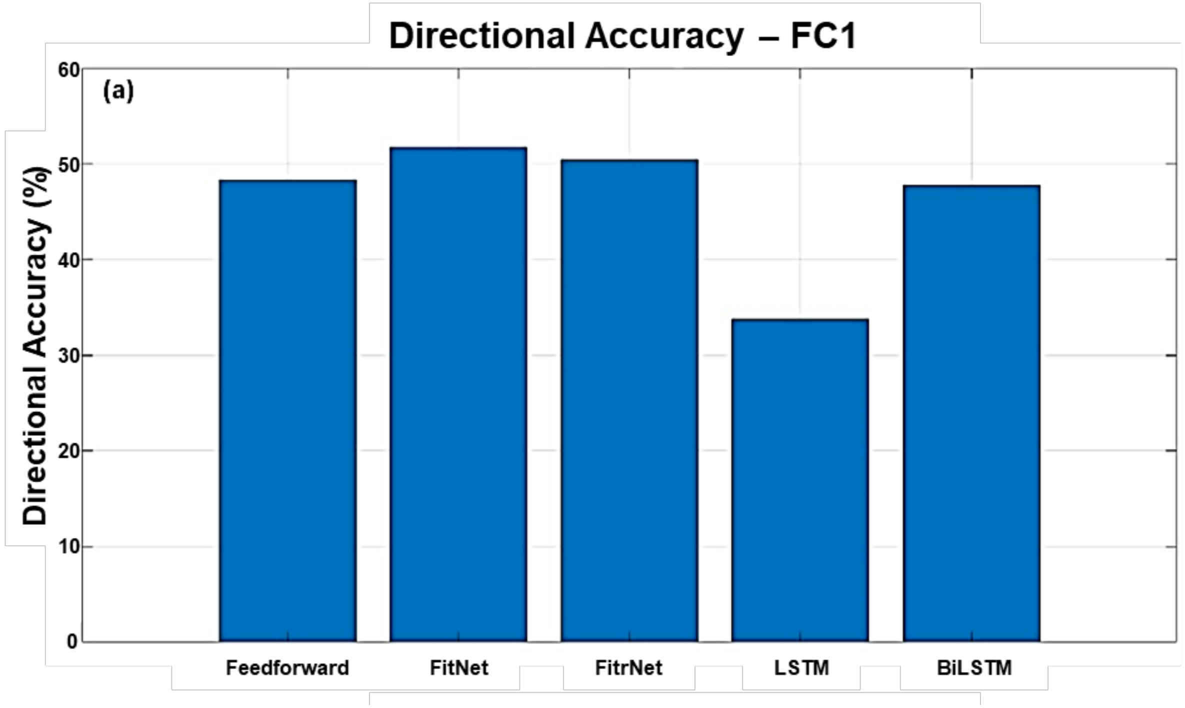

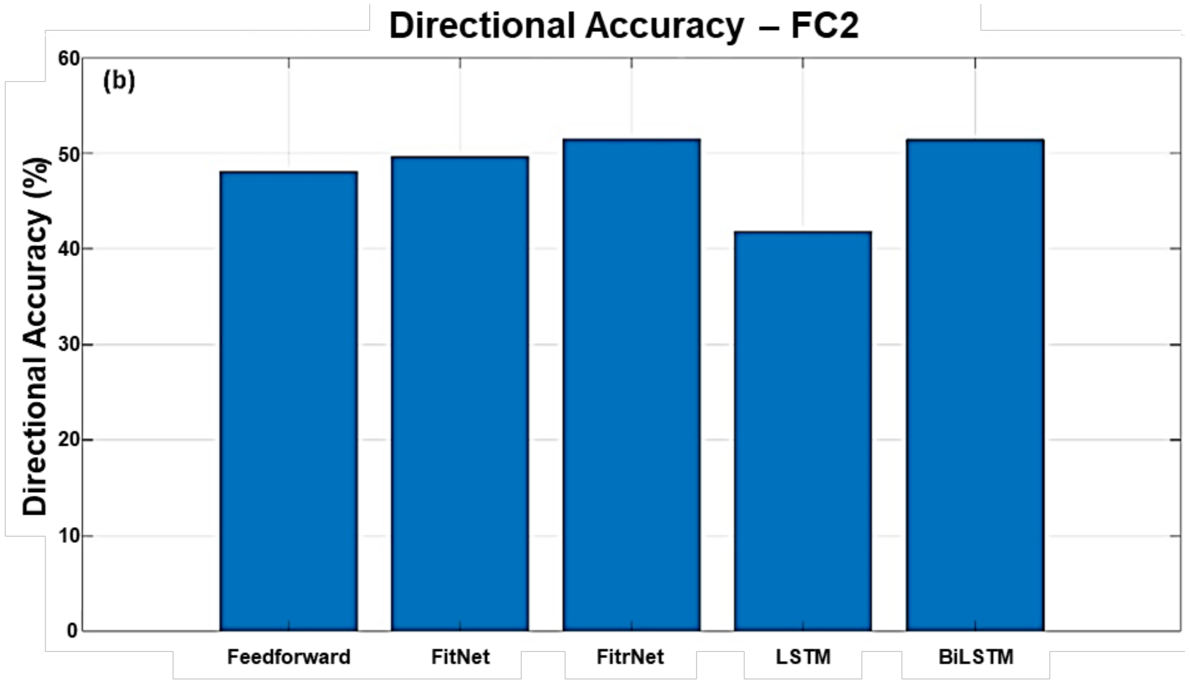

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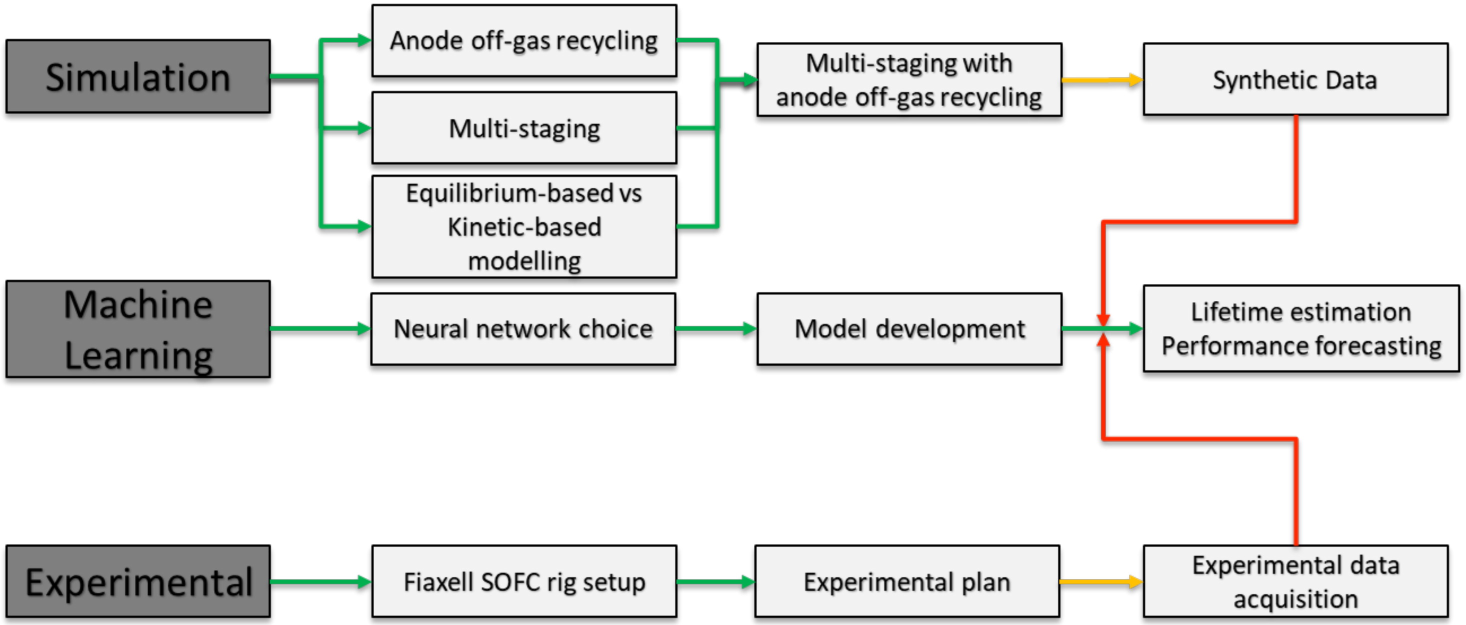
Experimental Work



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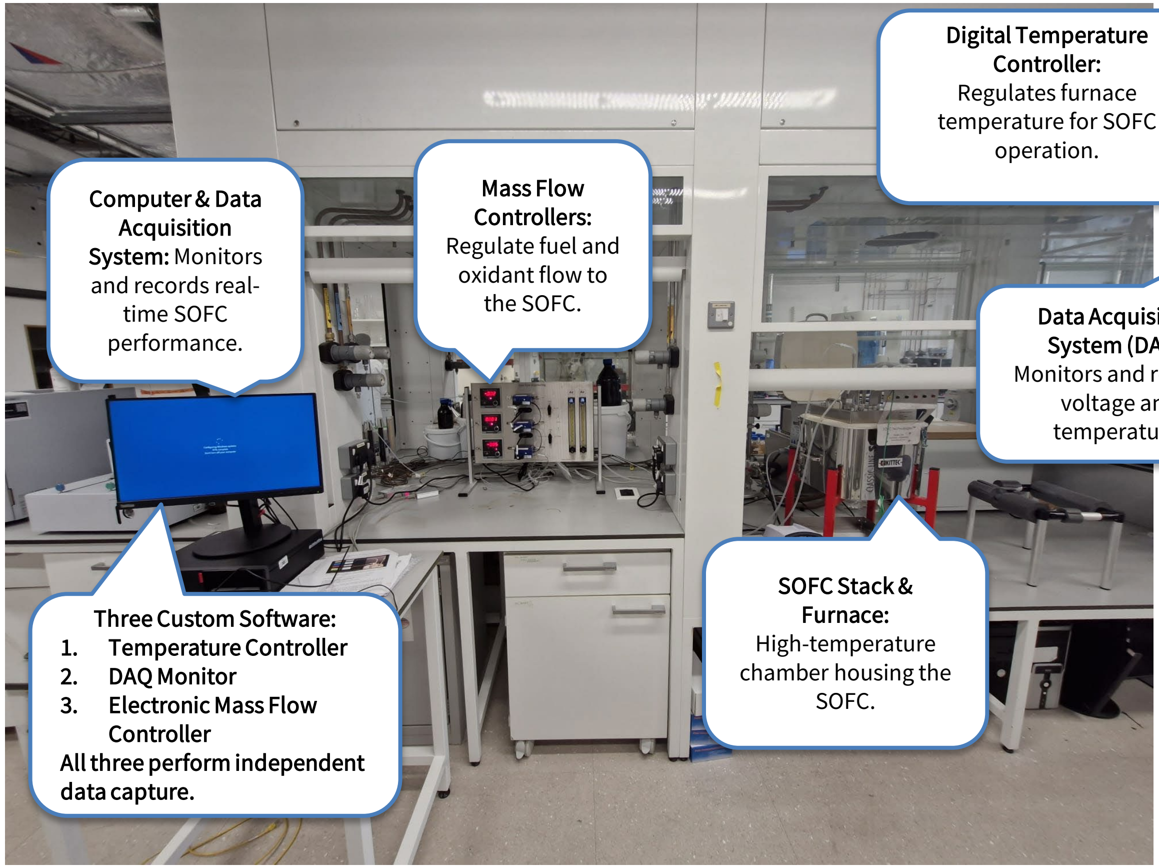
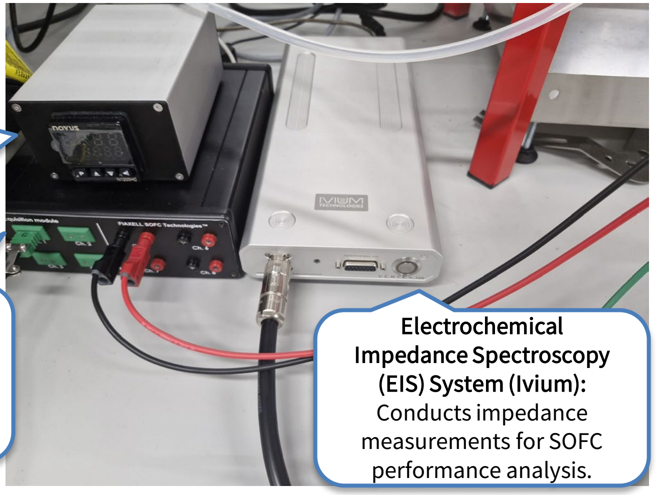
Experimental Work

Experimental → **Fiaxell SOFC Commissioning** → **Experimental plan** → **Operational data acquisition**





The SOFC test rig includes:

- A temperature controller for precise thermal regulation.
- A data acquisition system (DAQ) for real-time monitoring.
- An electrochemical impedance spectroscopy (EIS) unit for advanced performance diagnostics.
- Supports both single-cell and short-stack configurations.
- Can operate with either pure hydrogen or methane as fuel.

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Experimental Work: Future Plans

Experimental → **Fiaxell SOFC Commissioning** → **Experimental plan** → **Operational data acquisition**

- Clearly demonstrate system performance degradation over time.
- Cover multiple operating modes.
- Include multiple scenarios (e.g., thermal cycling, dynamic loading).
- Provide data sufficient to extract reaction kinetics and degradation rates.

*Industrial standards **typically require 40,000–90,000 hours** of operational data for accurate kinetic modelling. However, for laboratory-based accelerated degradation studies, approximately 4,000 hours should be sufficient to develop conceptual models.*

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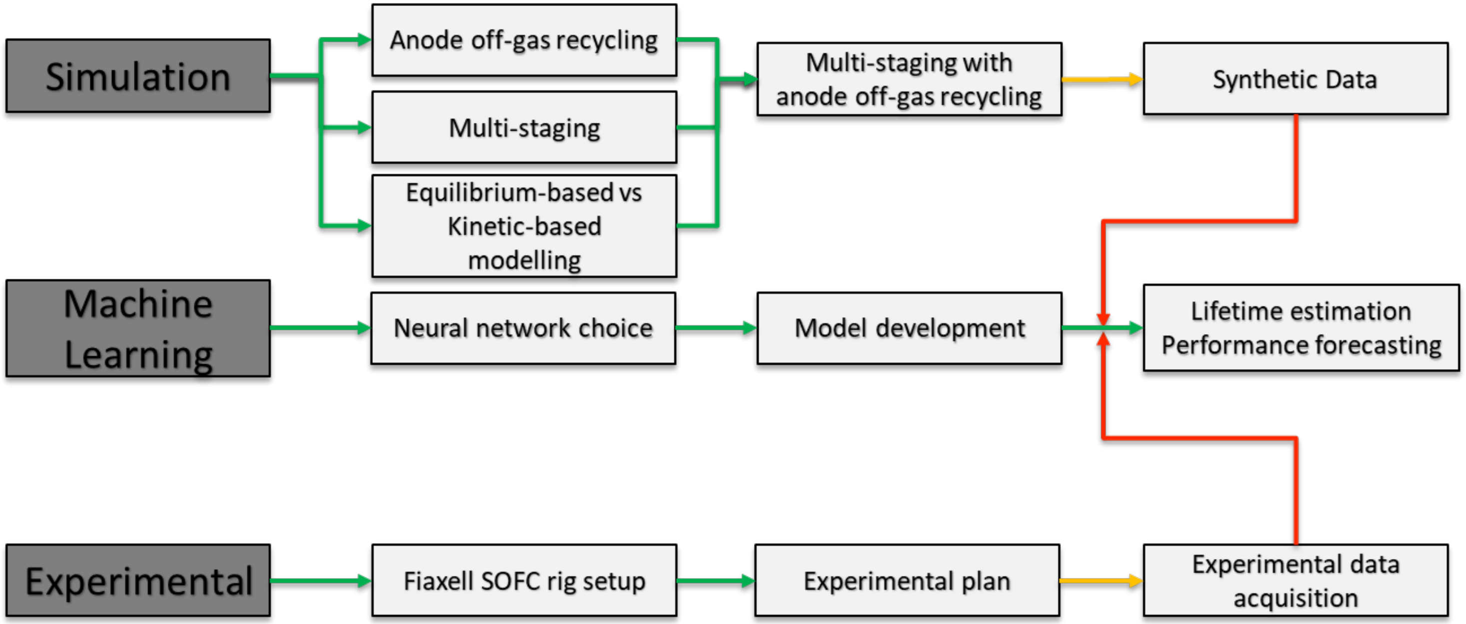
RESEARCH OVERVIEW



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Thank you!

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