Electrochemical Modelling and Experimental Validation of Proton Exchange Membrane Water Electrolysers for Loss Decomposition and Techno-Economic Assessment

Haotian MA

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Catalina Spataru

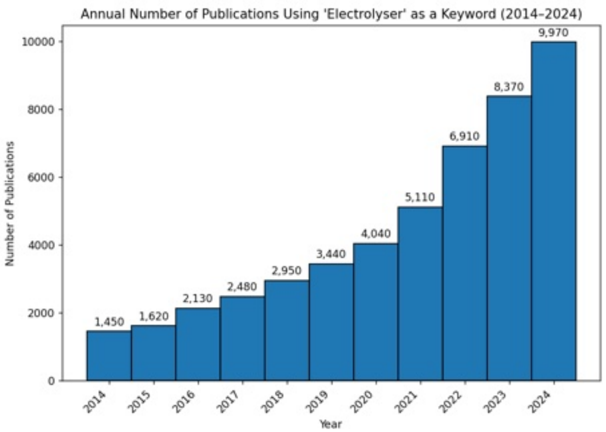
2025.06.20

University College London (2025)

RESEARCH BACKGROUND – RISING TRENDLINE

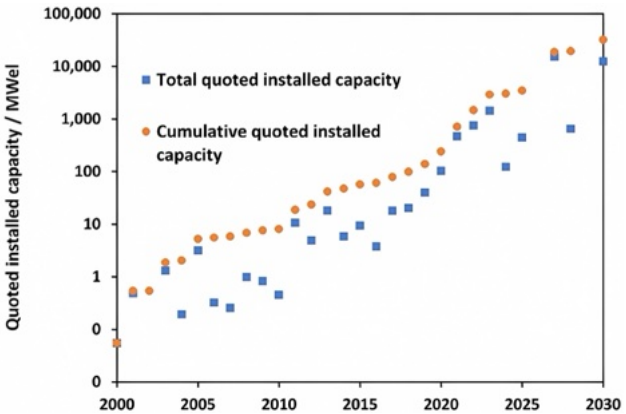
Schematics and projections illustrating the working principle and global scaling of electrochemical technologies.

Research



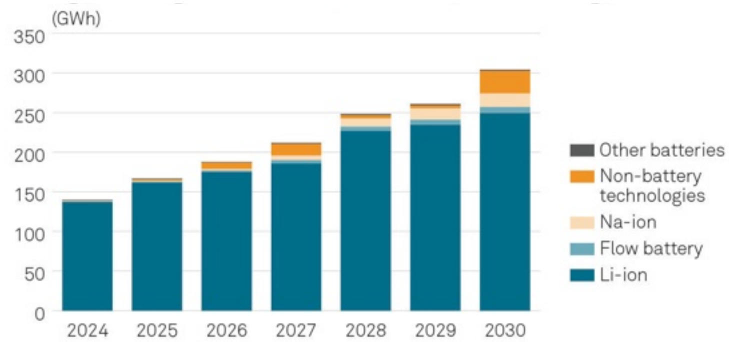
(a). Publication Numbers of Proton Exchange Membrane (PEM) Water Electrolysers from Google Scholar

Application



(b). Quoted Installed Capacity;

Projection



(c). Global Electrochemical Energy Storage Capacity by Classification, 2024–2030 (GWh);

Trends in PEM Electrolyser Research, Installed Capacity, and Global Electrochemical Energy Storage Production Capacity Prediction

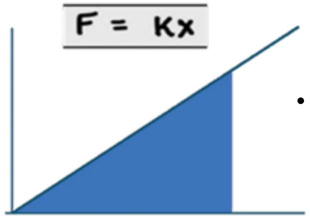
Reksten, A. H., et al. Int. J. Hydrogen Energy 47.96 (2022): 41015–41031.
Taylor, S., and Ribeiro, H. *Commodity Insights Magazine*. May 2024.

Identifiability vs. Uncertainty: A Modelling Dilemma

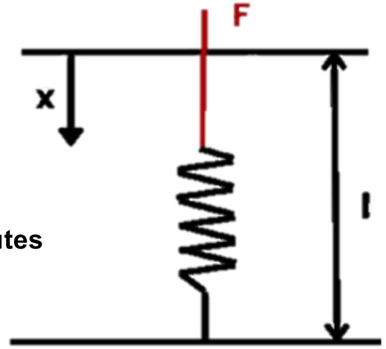
- Compare: Model g(ø) ↔ Experimental Data y_{exp}

Simple – Hooke's Law

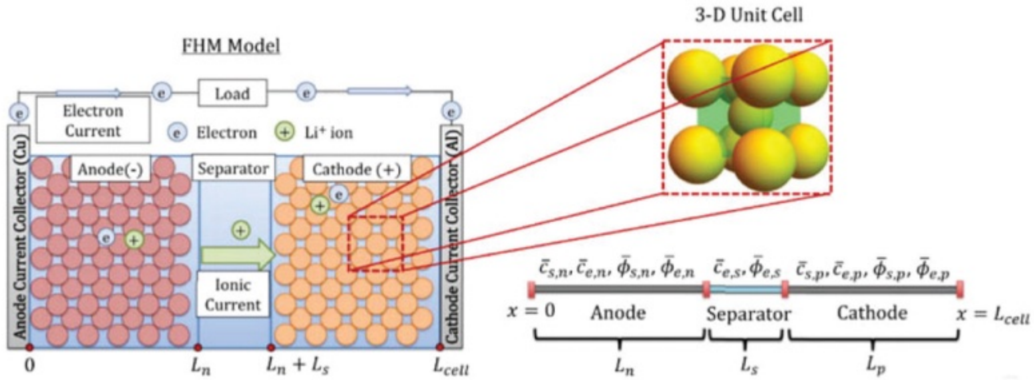
F = mg
= ρVg



- Simplified Metrics
- Linear Physical Attributes



Hard – Electrochemical System Modeling

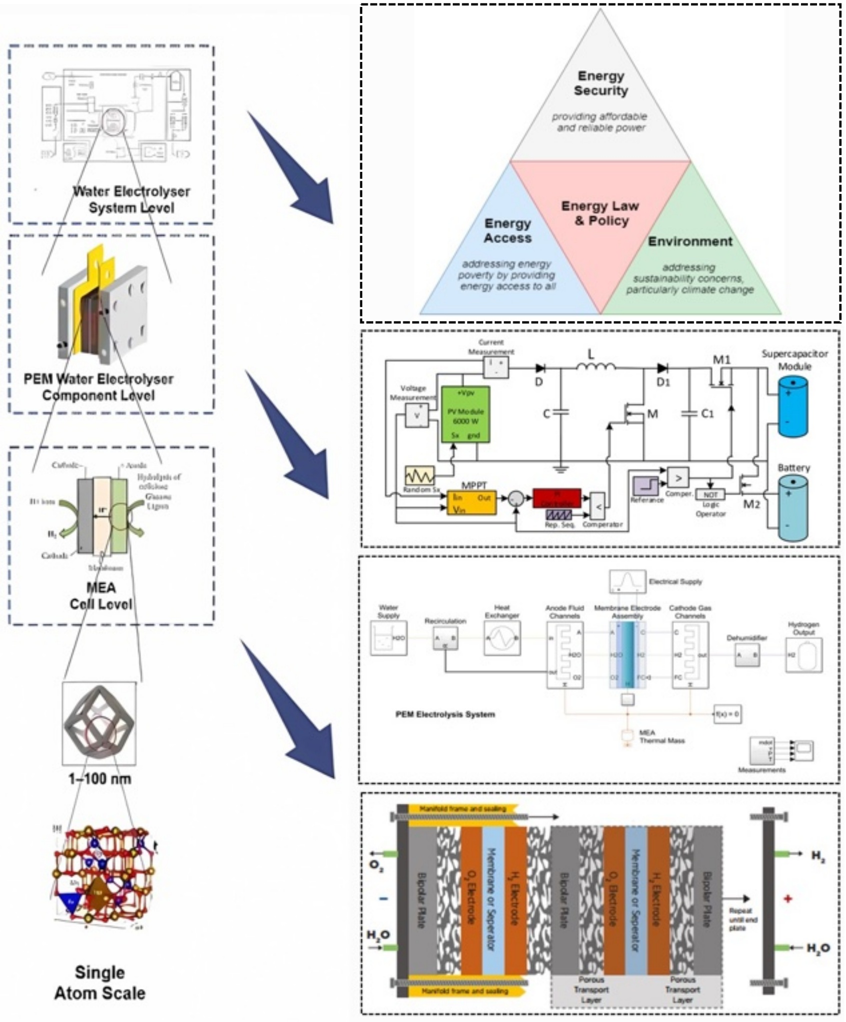


- High Dimensional Parameters Space → • Model Parametrization 
- Parameter Identifiability  → • Sensitivity Analysis 
- Experiment Noise
- Epistemic & Aleatory Uncertainty

} → • Uncertainty Quantification 

Khalik, Z., et al. *J. Power Sources* 499 (2021): 229901.

PEM-Integrated Hybrid Energy Storage Modelling and Optimization for Data Centre Resilience



Agenda:

a). Nature of electrochemical process scaling, and how it influences energy system design?

b). How does **multiscale modelling** link cell-level physics with system-level assessment?

c). How is the **data-driven framework applied** to calibrate and evaluate electrochemical subsystems?

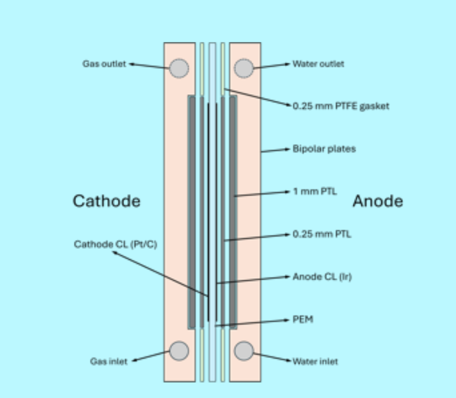
d). How are validated subsystem models integrated with **real-world** load and PV profiles in data centre simulations?

e). What does **resilience** mean in data centre and how can HESS support it?

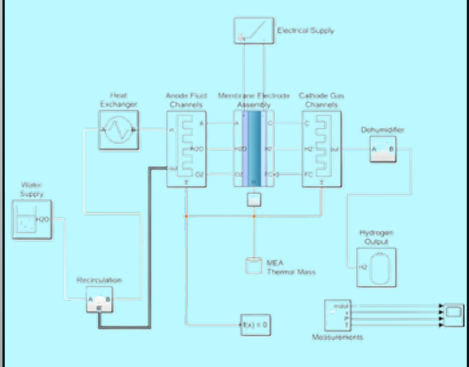
f). How does scenario-based optimization shape HESS sizing and control decisions?

OUTLINE

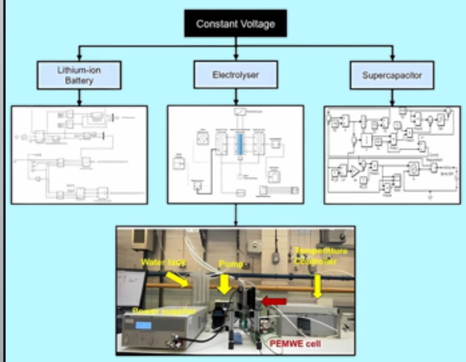
Experimental Setup



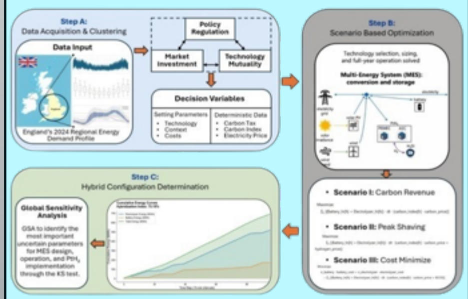
Electrode Simulation



HESS Process Modelling



System Sizing



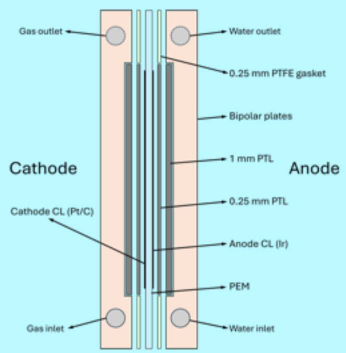
S1: Experimental Setting-up and Testing Benchmark

Experimental Setup

Electrode Simulation

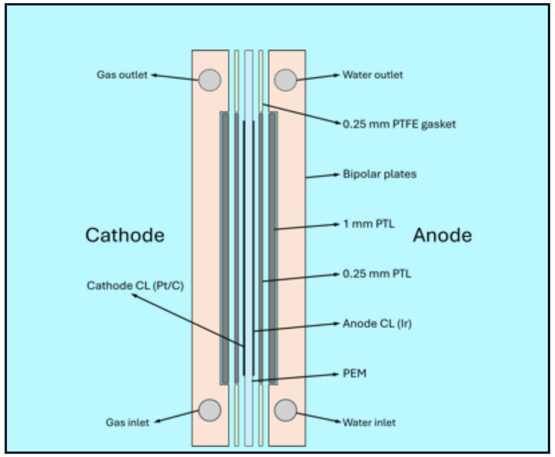
HESS Process Modelling

System Sizing

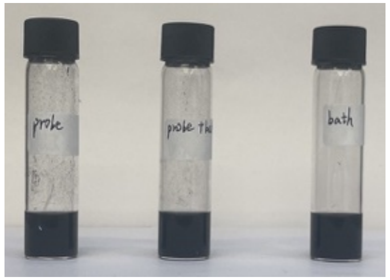


- Experimental Setting-up and Lab Overview @ University of Birmingham

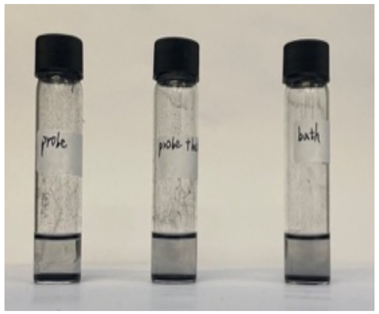
Materials Preparation



(1). Ink Preparation

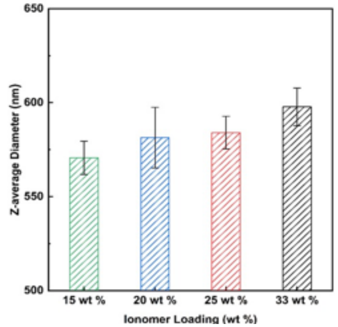


Photograph of Catalyst Ink before Sonication Methods

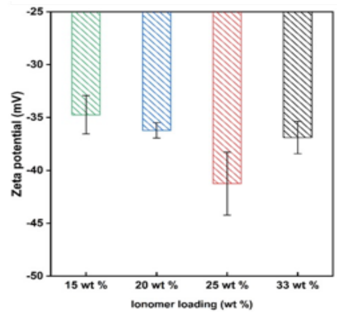


Photograph of Catalyst Ink after Sonication Methods(@210 min)

(2). Dispersion Properties

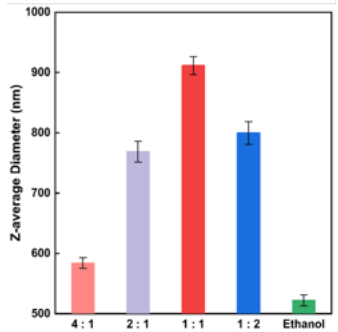


Effect of Ionomer Content on Catalyst Ink Particle Size

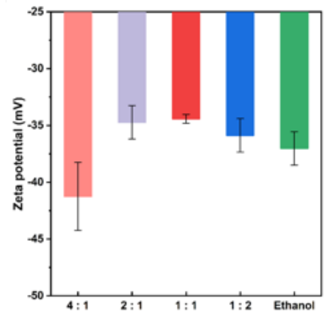


Zeta Potential of Catalyst Ink with Varying Ionomer Loadings

(3). Electrode Structure



Size distribution of Ir inks (IPA:H_2O varied, EtOH:H_2O = 4:1)



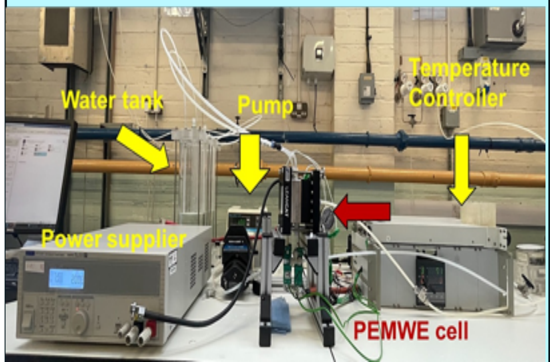
Zeta potential of Ir inks (same conditions)

Hou, D., et al. *Chem. Eng. J.* **512** (2025): 162524.

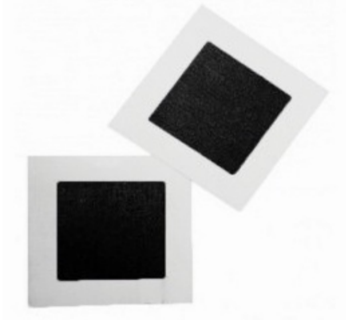
Workflow for Electrochemical Evaluation

- MEA Fabrication and Testing Procedure

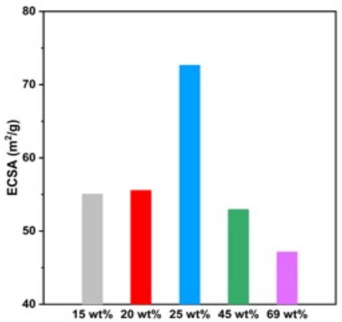
Testing Station Setting-up



(4). Membrane Electrode Assembly Fabrication

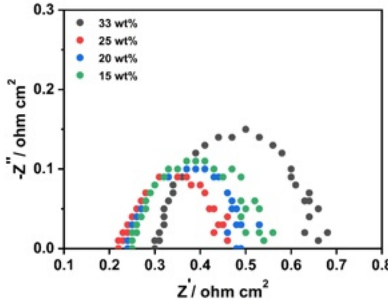


Photograph of Catalyst-Coated Membranes

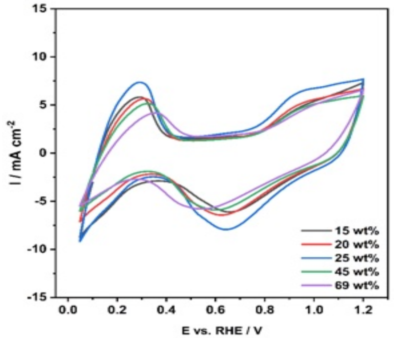


Electrochemical Surface Area (ECSA)

(5). Electrochemical Performance

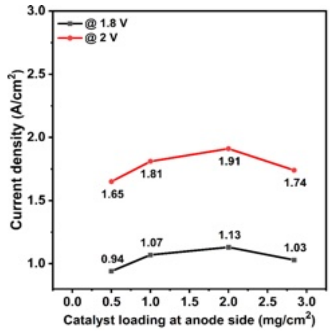


Electrochemical Impedance Spectra of Electrodes

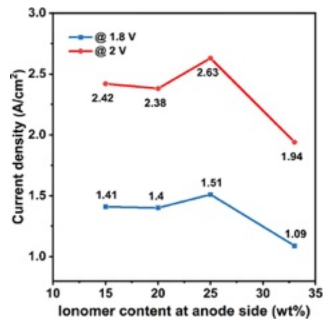


Cyclic Voltammetry of Electrodes

(6). Performance Benchmarking



Current density with varying anode ionomer content

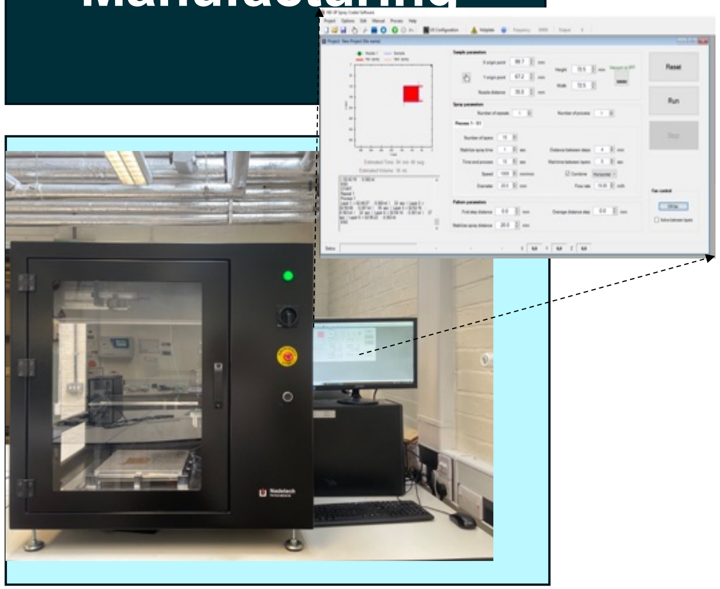


Current density with varying anode catalyst loading

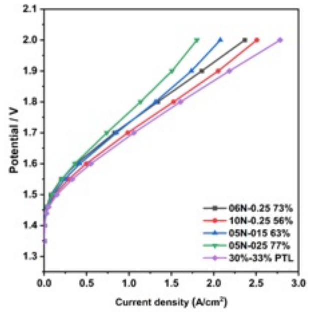
Hou, D., et al. *Chem. Eng. J.* **512** (2025): 162524.

- Sensitivity Analysis and Scaling up Testing

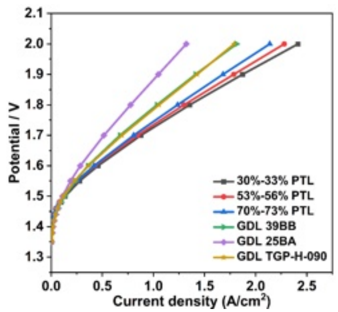
Additive Manufacturing



(a). PTL Selection

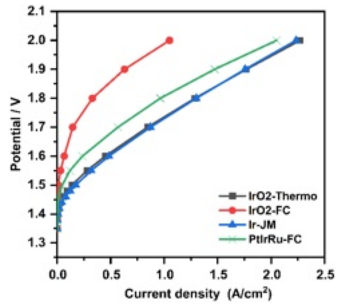


Effect of Anode PTLs on I–V Characteristics

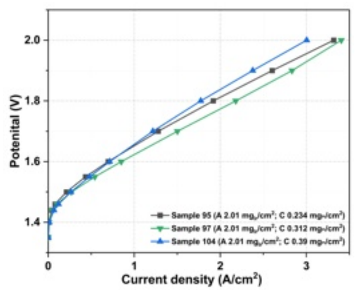


Effect of Cathode PTLs on I–V Characteristics

(b). Catalyst Selection

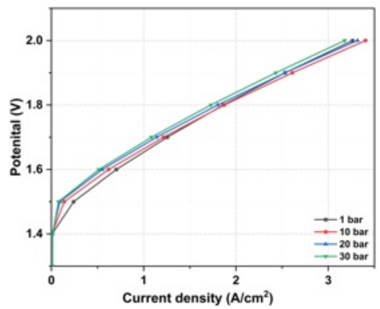


Effect of OER Catalyst Type on I–V Characteristics

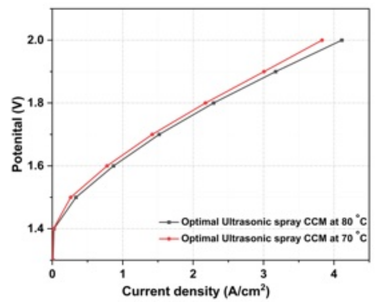


Effect of Cathode Catalyst Loading on I–V Characteristics

(c). Engineering Parameters



Effect of Cathode Pressure on I–V Characteristics



Effect of Testing Temperature on I–V Characteristics

Hou, D., et al. *Chem. Eng. J.* **512** (2025): 162524.

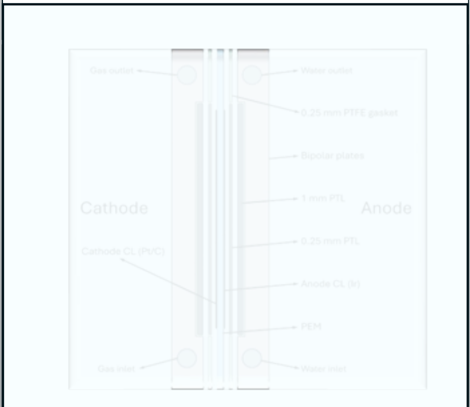
S2: Electrolyser Electrochemical Subsystem Modelling

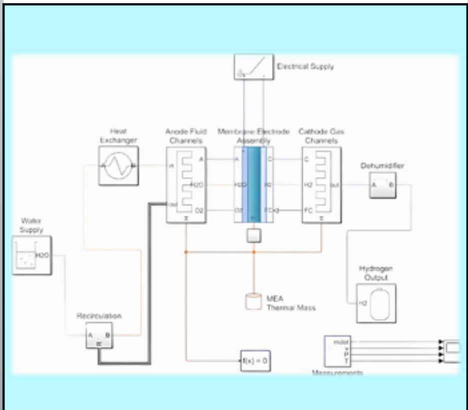
Experimental Setup

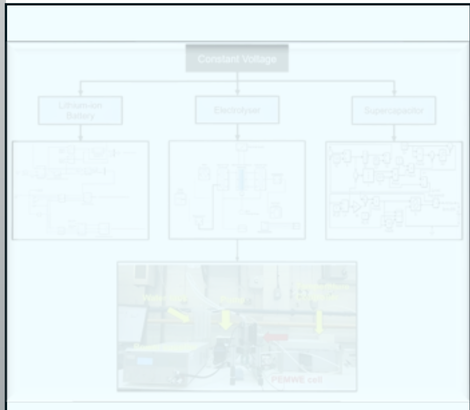
Electrode Simulation

HESS Process Modelling

System Sizing



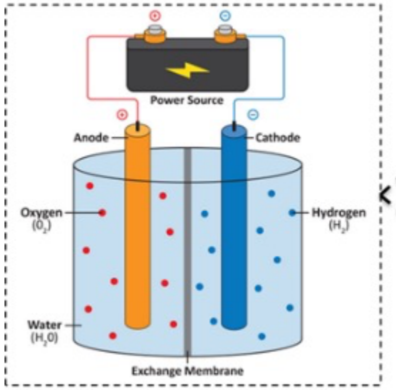




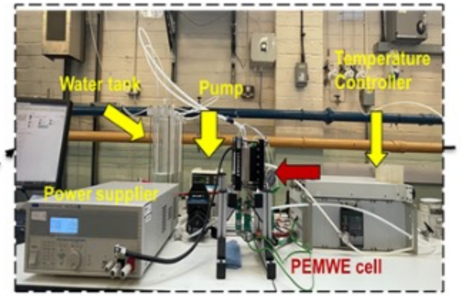
Overall Methodology for Electrochemical Modelling & Experimental Validation

Voltage Decomposition and Parametric Modelling of PEM Electrolyser Cells

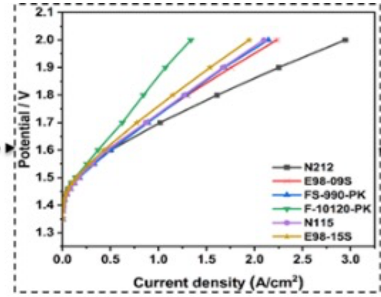
- $S = \{A:[J_a, \eta_a], C:[J_c, \eta_c], P:[p_{an}, p_{ca}], T:[T_1, T_2]\}$*



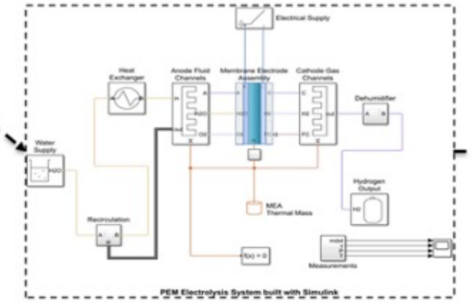
(a). Schematic of the electrochemical reaction mechanism



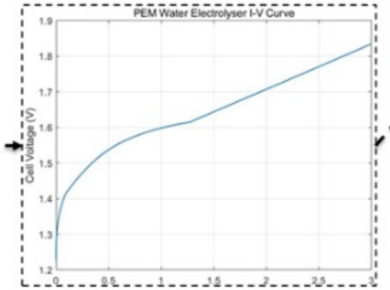
(b). Experimental setup with PEM cell



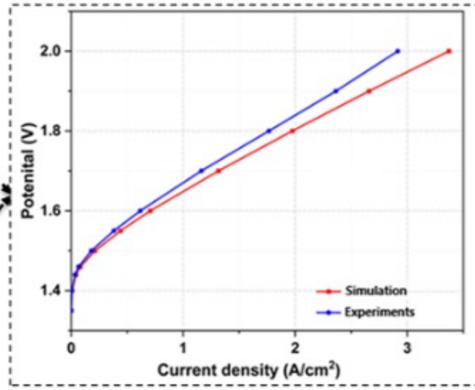
(c). Polarization curves for different membranes



(d). MATLAB/Simulink Simscape model of the system



(e). Simulated polarization curve using calibrated parameters



(f). Comparison between simulation and experiment

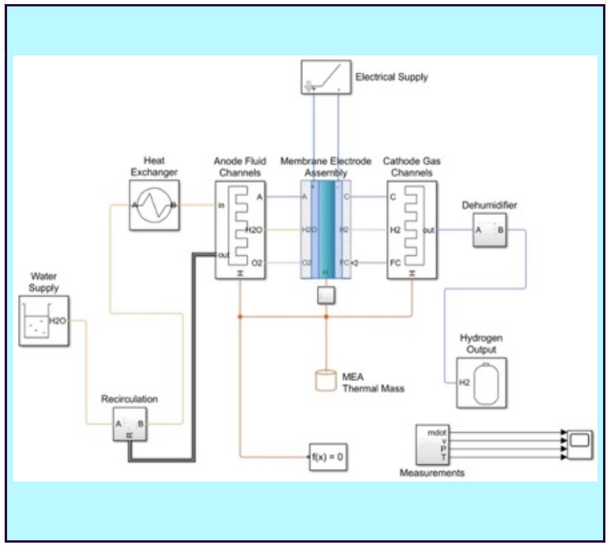
Integrated Methodology for Electrochemical Modelling, System Simulation, and Experimental Validation of PEM Water Electrolyser Subsystem

*A : Anode; C:Cathode;P:Pressure: T:Temperature

Modular Gas & Water & Thermal Management in Electrochemical System Modelling

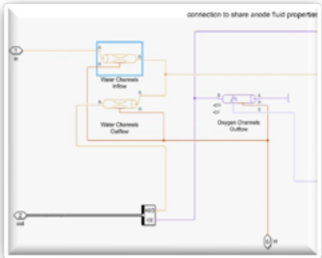
- System S ↔ {A:[a_1,a_2], C:[c_1,c_2], P:[p_1,p_2], T:[t_1,t_2]}

Electrochemical System Simulation

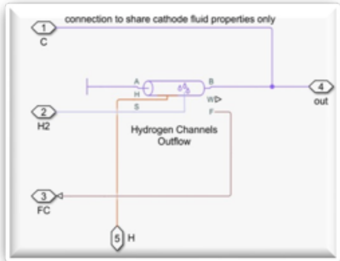


Core Process

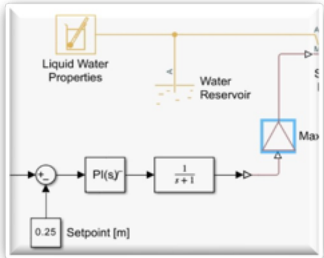
(1).Anodic Gas Management	(2).Cathodic Gas Management	(3).Phase Separation	(4).Thermal & Moisture Regulation



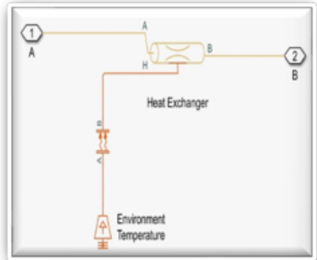
Anode Oxygen Generation Unit



Cathode Hydrogen Generation Unit

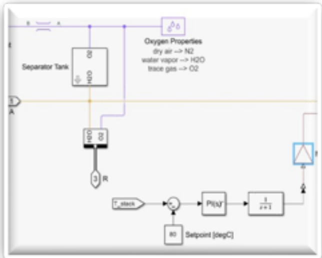


Water Circulation Unit

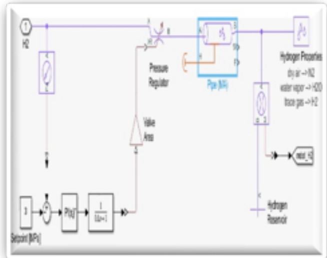


Thermal Management Unit

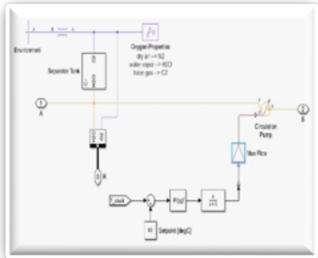
Supplementary System



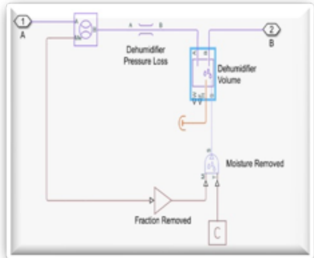
Water-Oxygen Balance & Venting Unit



Hydrogen Purification and Output Unit



Water-Gas Separation Unit

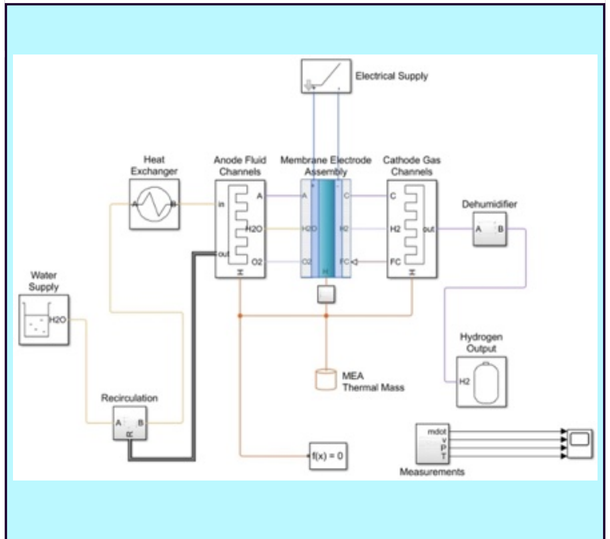


Hydrogen Dehumidification Unit

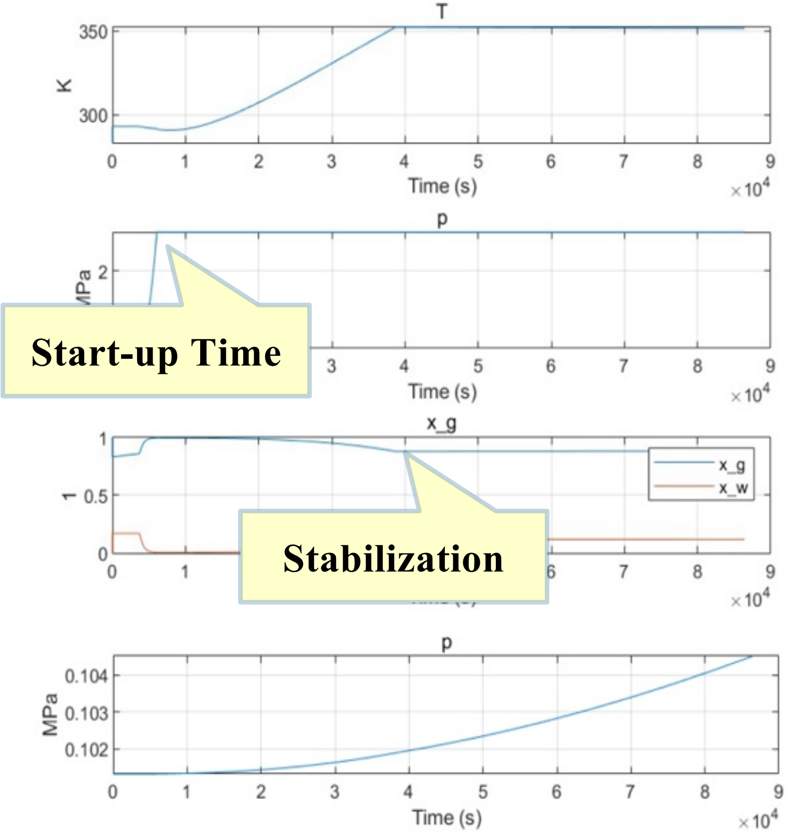
*A：Anode; C:Cathode;P:Pressure: T:Temperature

- Dynamical System Response and Performance Curve Fittings

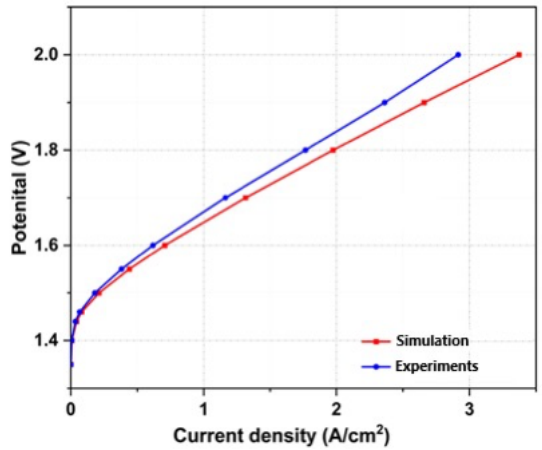
Electrochemical System Simulation

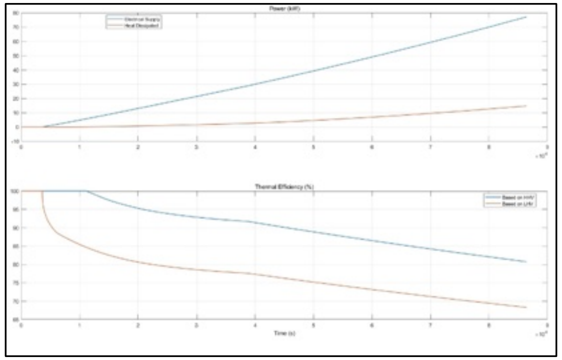


(1). Dynamic Simulation Results of PEM Electrolyser Under Variable Load Conditions



(2). System-level performance metrics



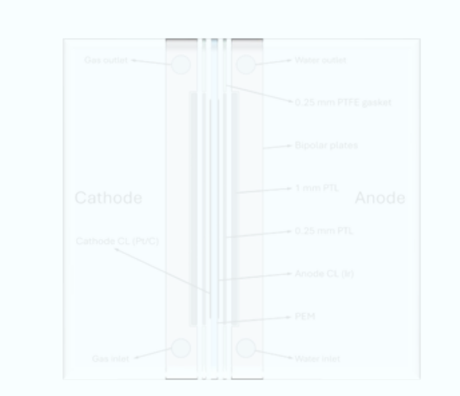


Li, Y., et al. *Int. J. Greenh. Gas Control* 130 (2024): 104112.

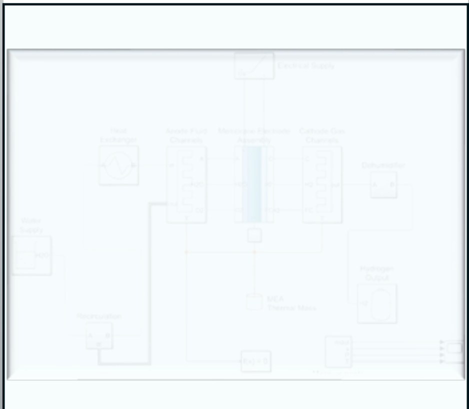
S3: Hybrid Electrochemical Energy Storage System Process Modelling

UCL

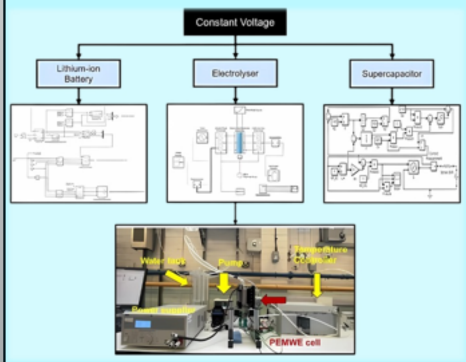
Experimental Setup



Electrode Simulation



HESS Process Modelling

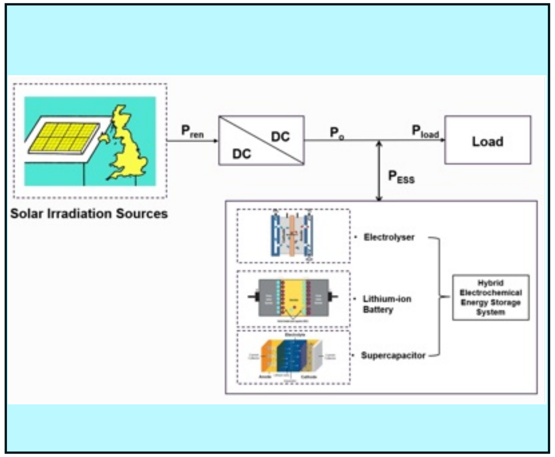


System Sizing

Hybrid Electrochemical Energy Storage System

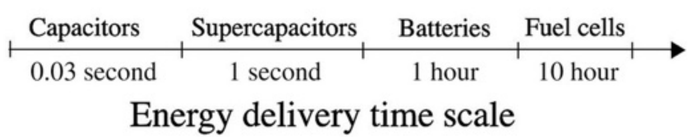
- Experimental Setting-up and Lab Overview @ University of Birmingham

Hybrid System Architecture Designing

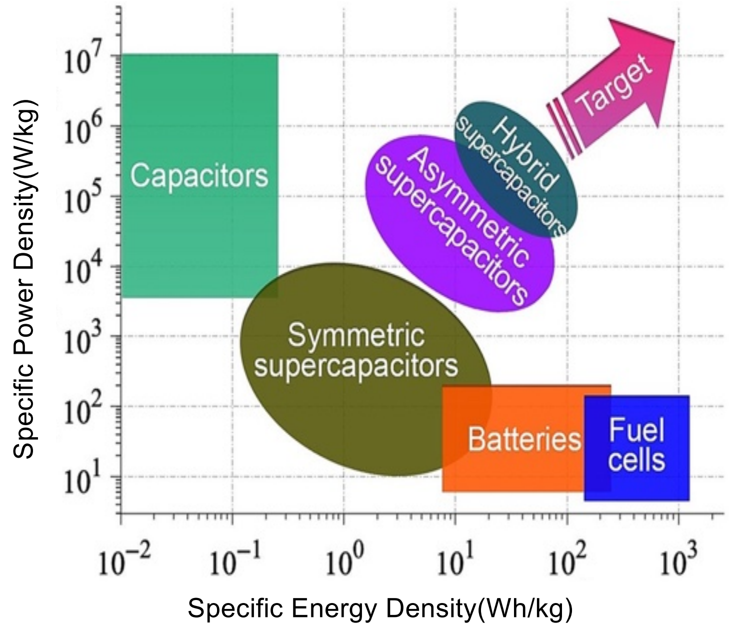


Candidate Selection

	Li-ion Battery	EDLC Supercapacitor
Recharge Cycle Life Time	< 10^3 cycles	> 10^6 cycles
Voltage	3.7V-4.2V	0V-2.7V
Energy Density (Wh/kg)	High(20-150)	Low(0.8-10)
Power Density (W/kg)	Low(50-300)	High(500-400)
Fastest Charging Time	Hours	Sec – Min
Fastest Discharging Time	0.3-3 hours	<a few min
Charging Circuit	Complex	Simple

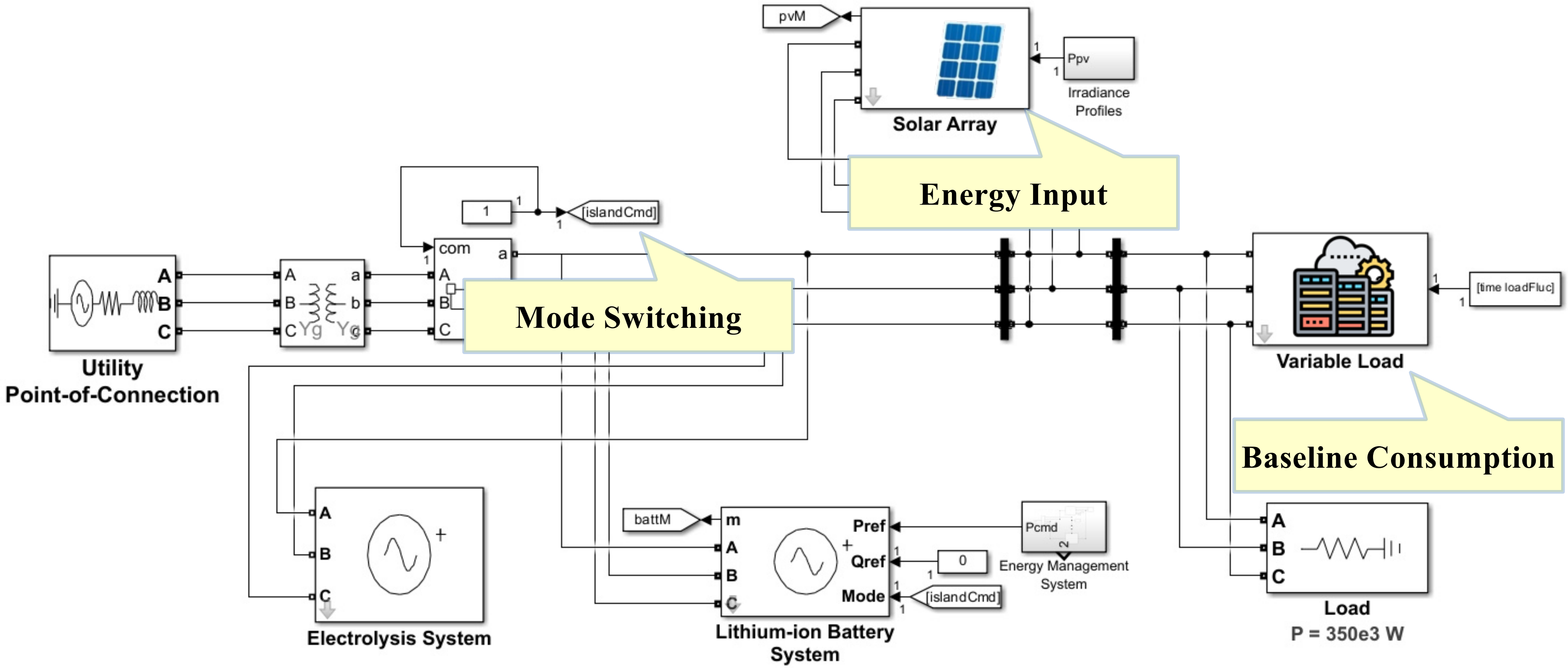


Target Hybrid Energy Systems



Zulfiqar, Z., et al. Energy Storage 6.1 (2024): e506.

- Architecture Designing of Hybrid Energy System

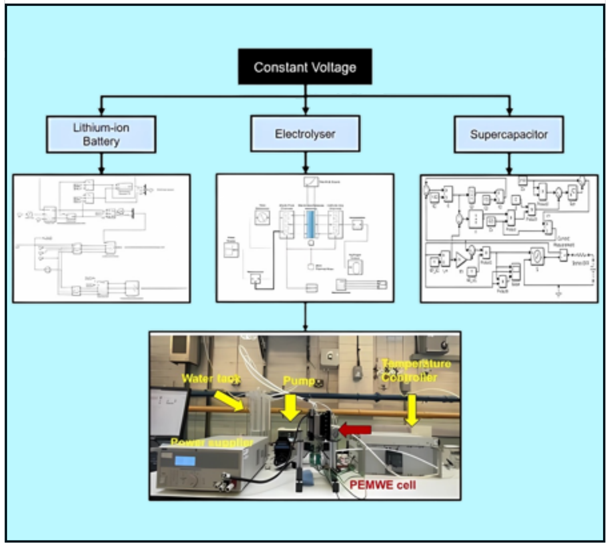


Hybrid Electrochemical Energy Storage System Architecture Design Using Simulink

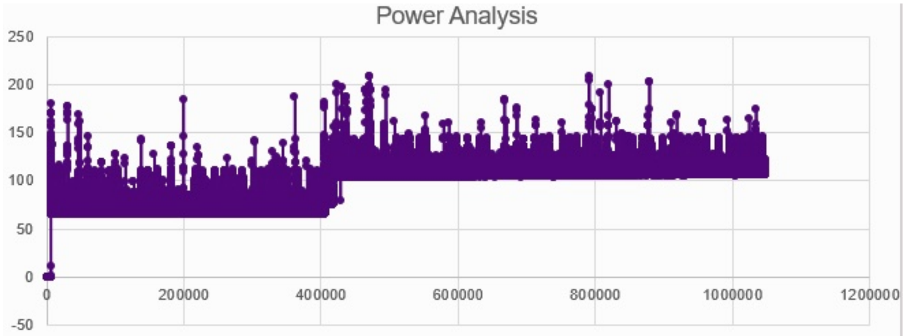
Ma, H., et al. IEEE GPECOM 2025 (2025).

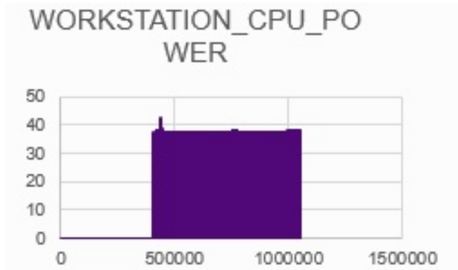
- Solar Energy Generation Profile and Data Centre Energy Consumption Profile

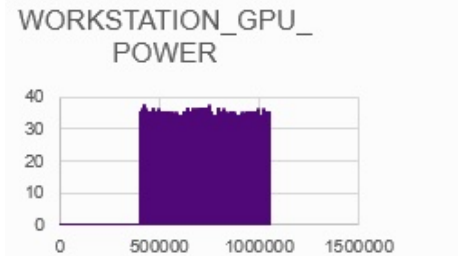
Electrochemical System Simulation



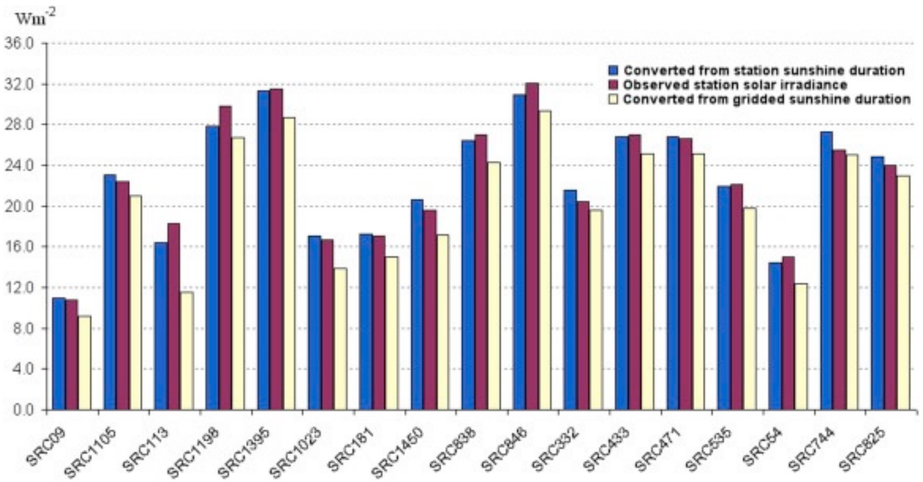
Battery Management

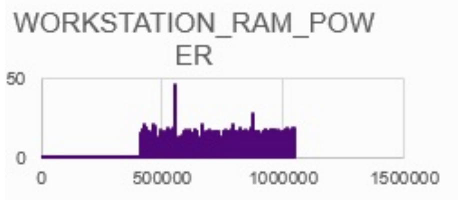






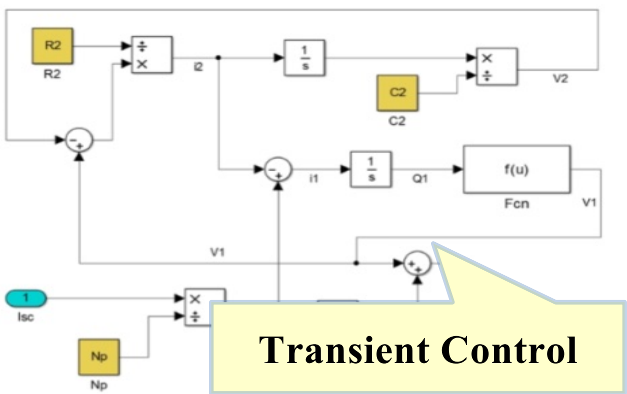
Power Analysis of Data Centre





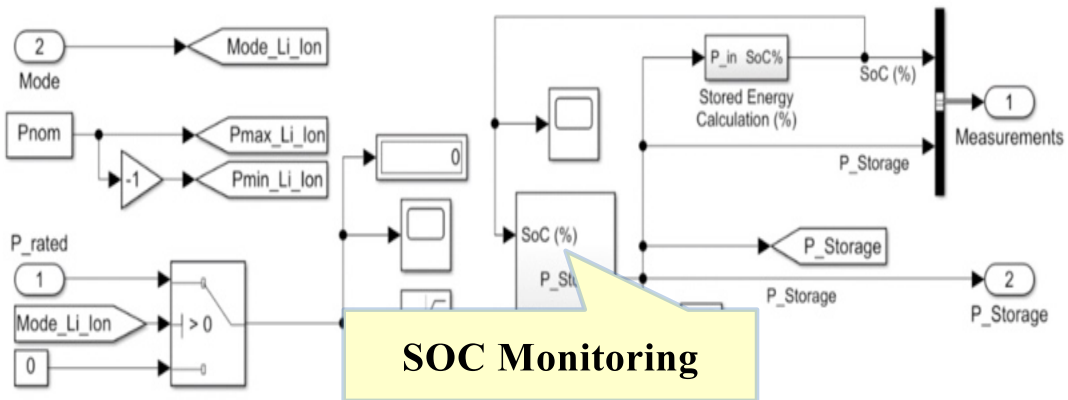
- Optimal Sizing of Hybrid Electrochemical Energy Storage Systems

EDLC Supercapacitor



(a).Simulink-based EDLC Supercapacitor Designing;

Lithium-ion Battery

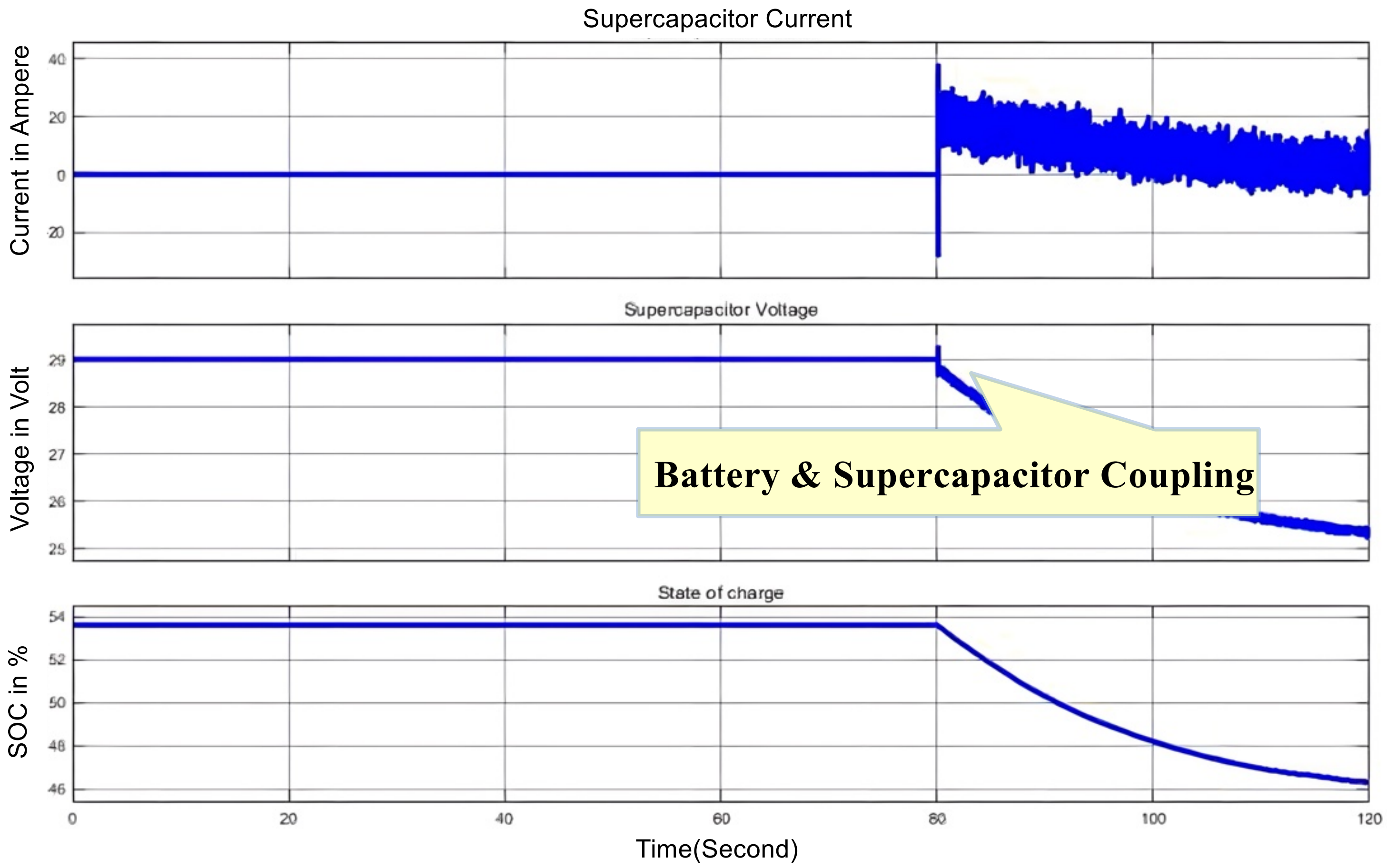


(b). Simulink-based Li-ion Battery Designing;

Hybrid Electrochemical Energy Storage Systems Designing

Möller & Krauter, Energies, 2022.
Arumugam C. et al., *High Energy Chem.*, 2025, 59(2), 101–106.

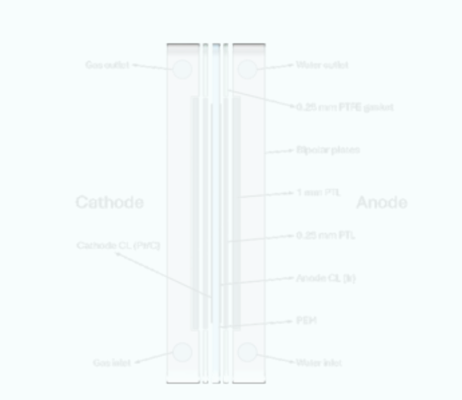
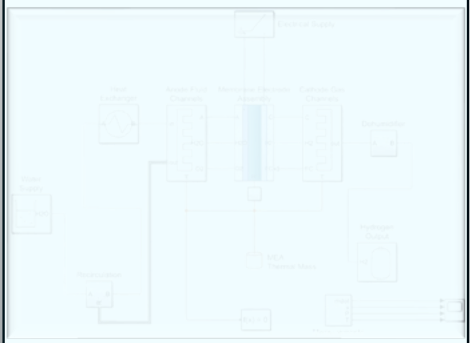
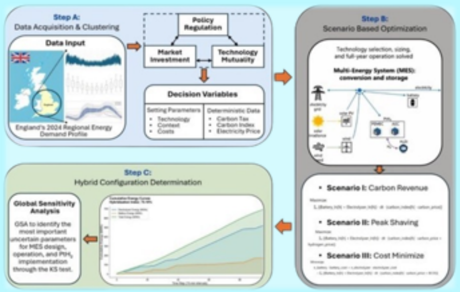
- HESS System Response and Performance Analysis

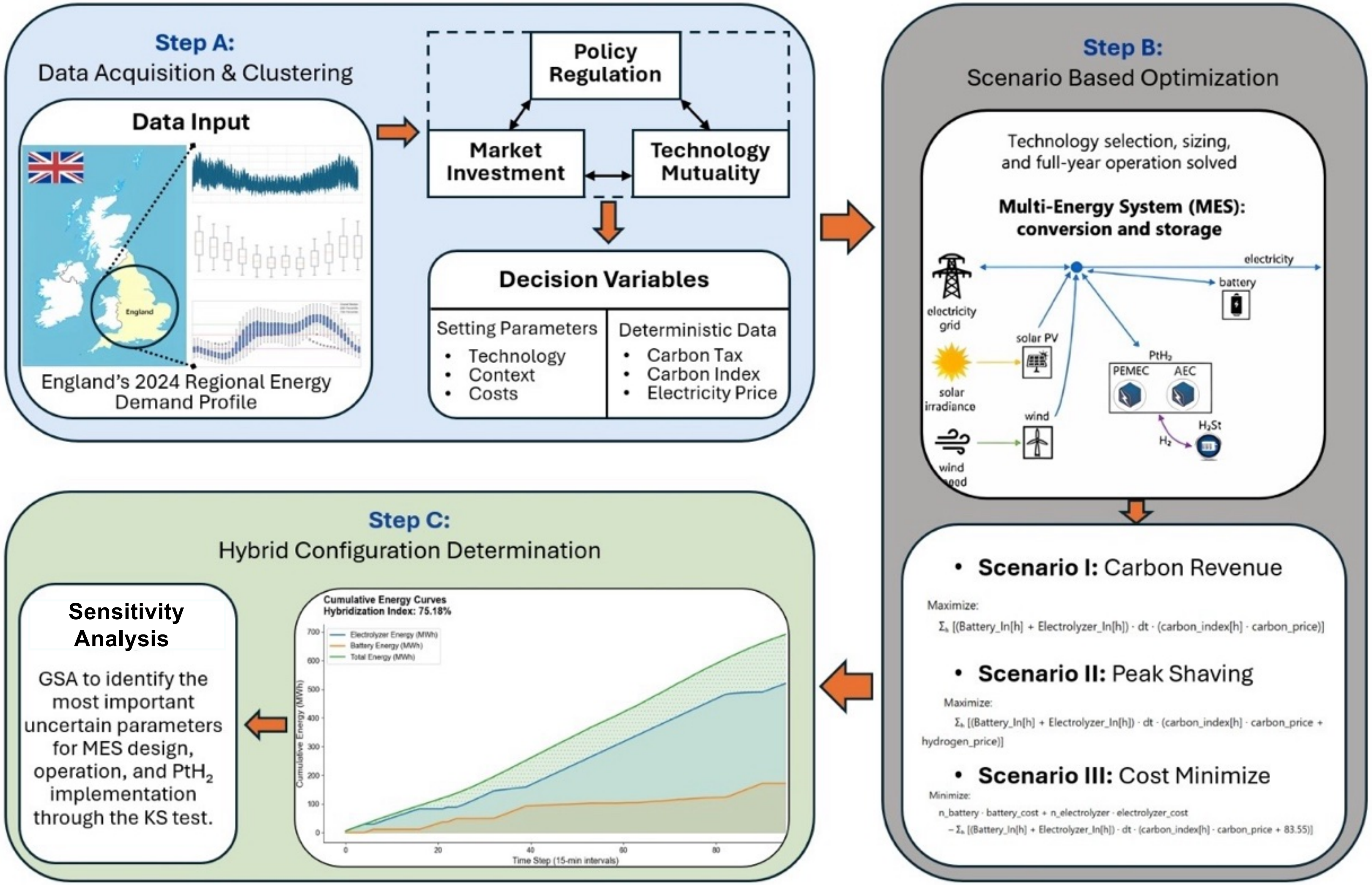


The control system has four modes:

- **Charging:** PV > load & SoC < 80% → battery charges
- **Discharging:** Load > PV & SoC > 20% → battery discharges
- **Hydrogen Production:** Battery & Supercapacitor full → excess PV powers electrolyser
- **Transient Response:** Supercapacitor buffers fast spikes (e.g., 5 kW in 50 ms) to stabilize voltage and protect the battery

S4: System Sizing and Optimisation

Experimental Setup	Electrode Simulation	HESS Process Modelling	System Sizing
			



Step A:

Data Acquisition & Preprocessing

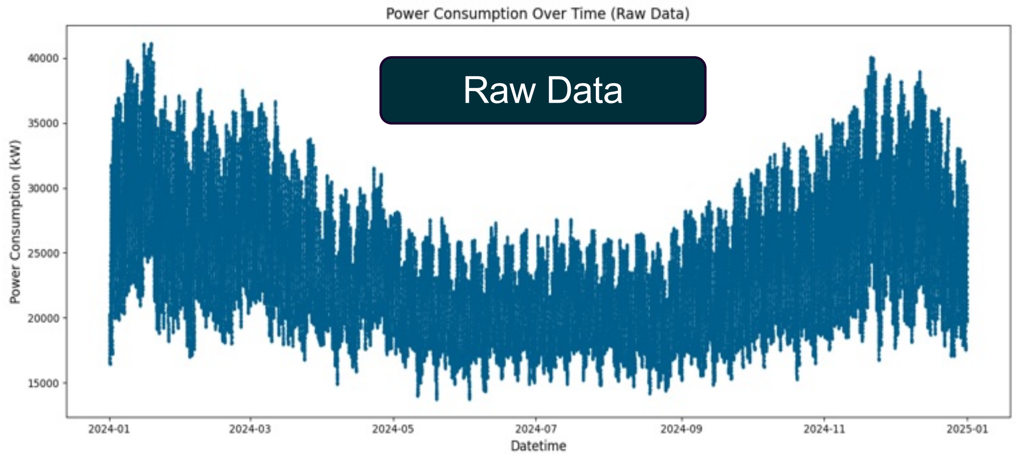
Step B:

Scenario Based Optimization

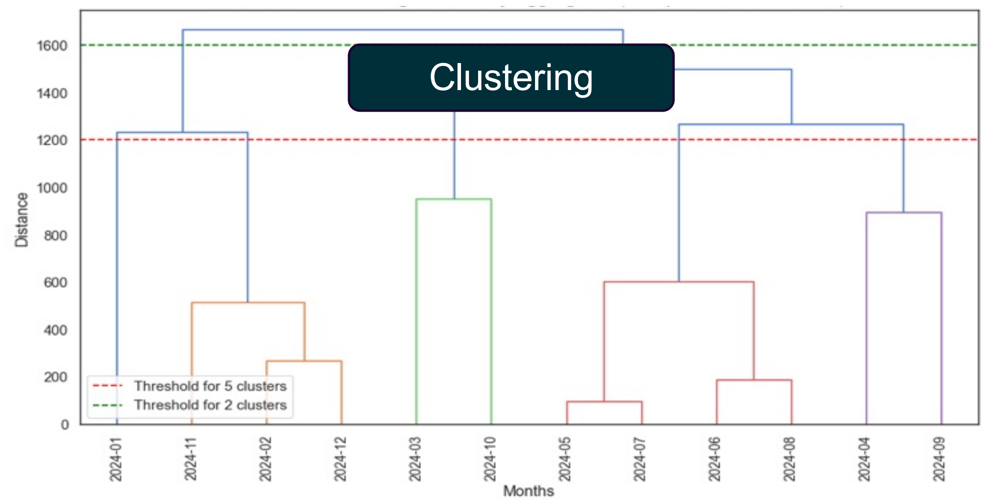
Step C:

Hybrid Configuration Determination

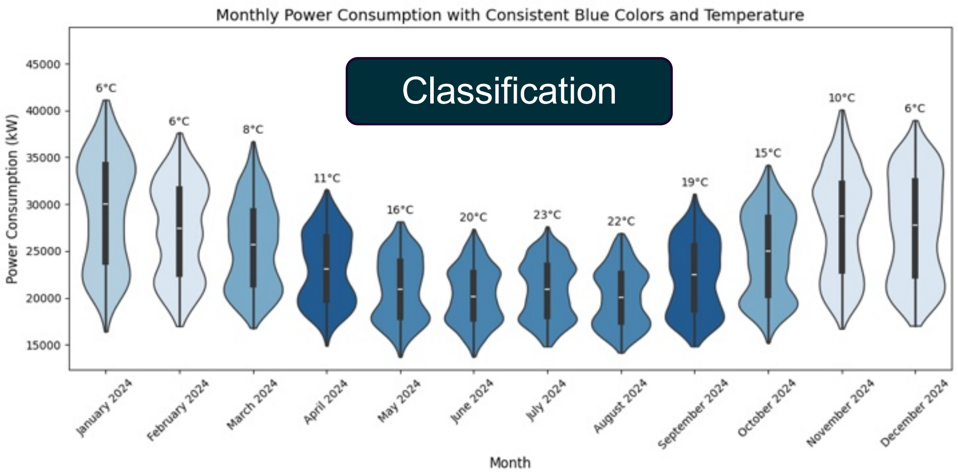
Power Distribution & Data Preprocessing



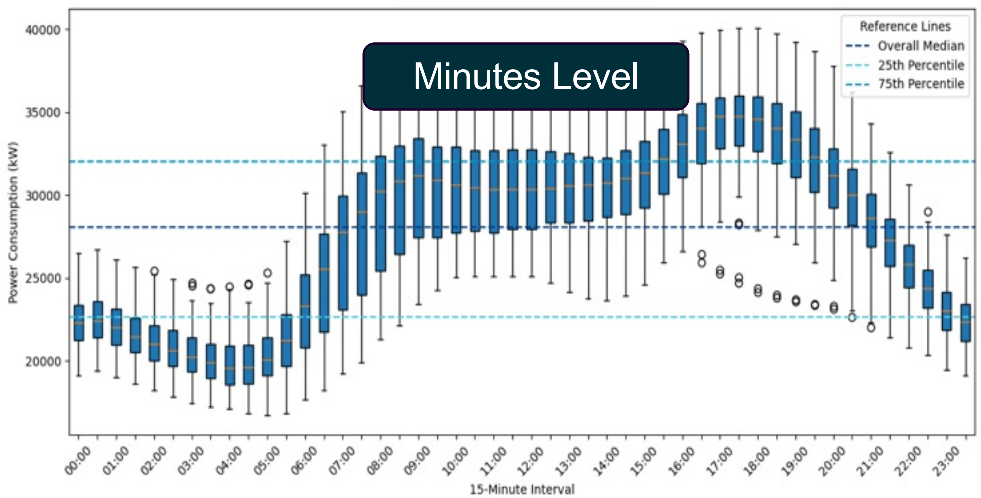
(a).Raw Data of Power Consumption



(b). Power Distribution Clustering

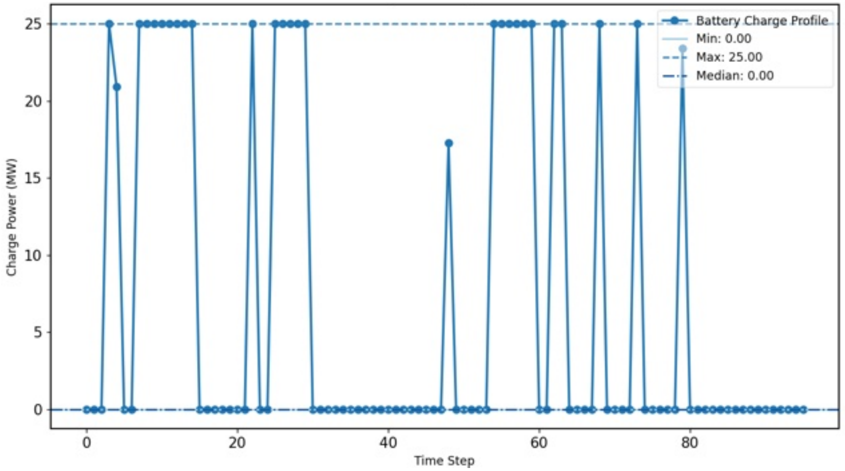


(c). Monthly Power Consumption Seasonal Classification

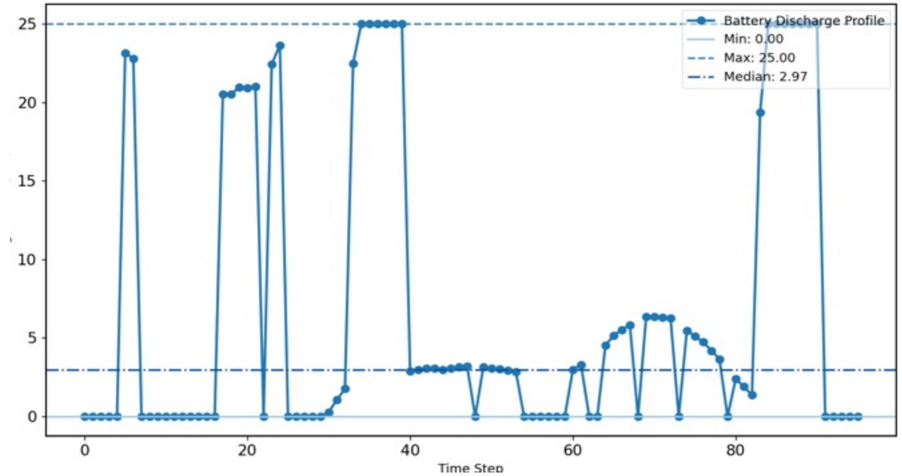


(d). Minutes Level Data Visualization;

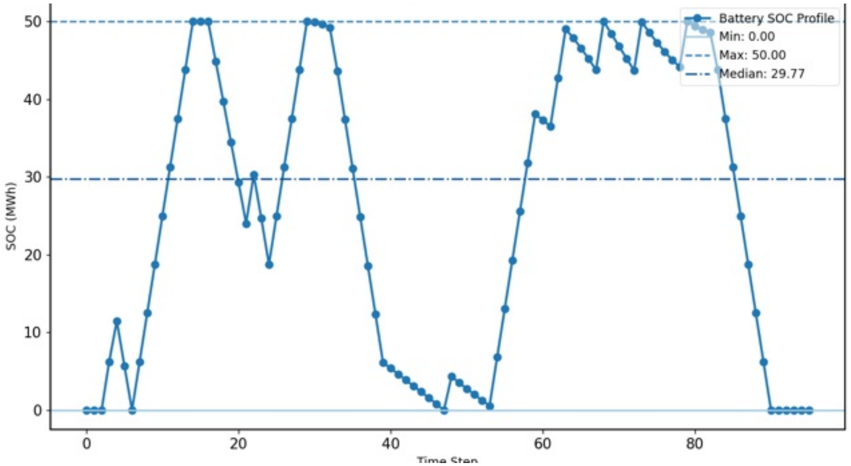
Battery & Electrolyser Performance Profile Under Given Scenario



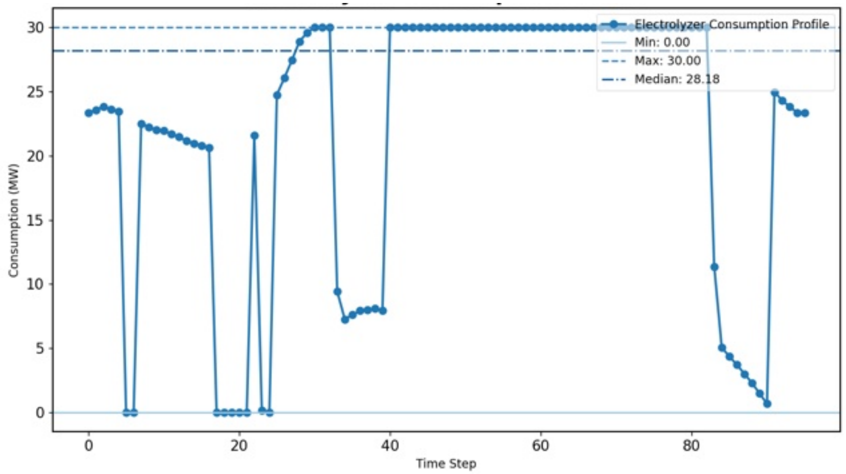
(a).Battery Charging Profile



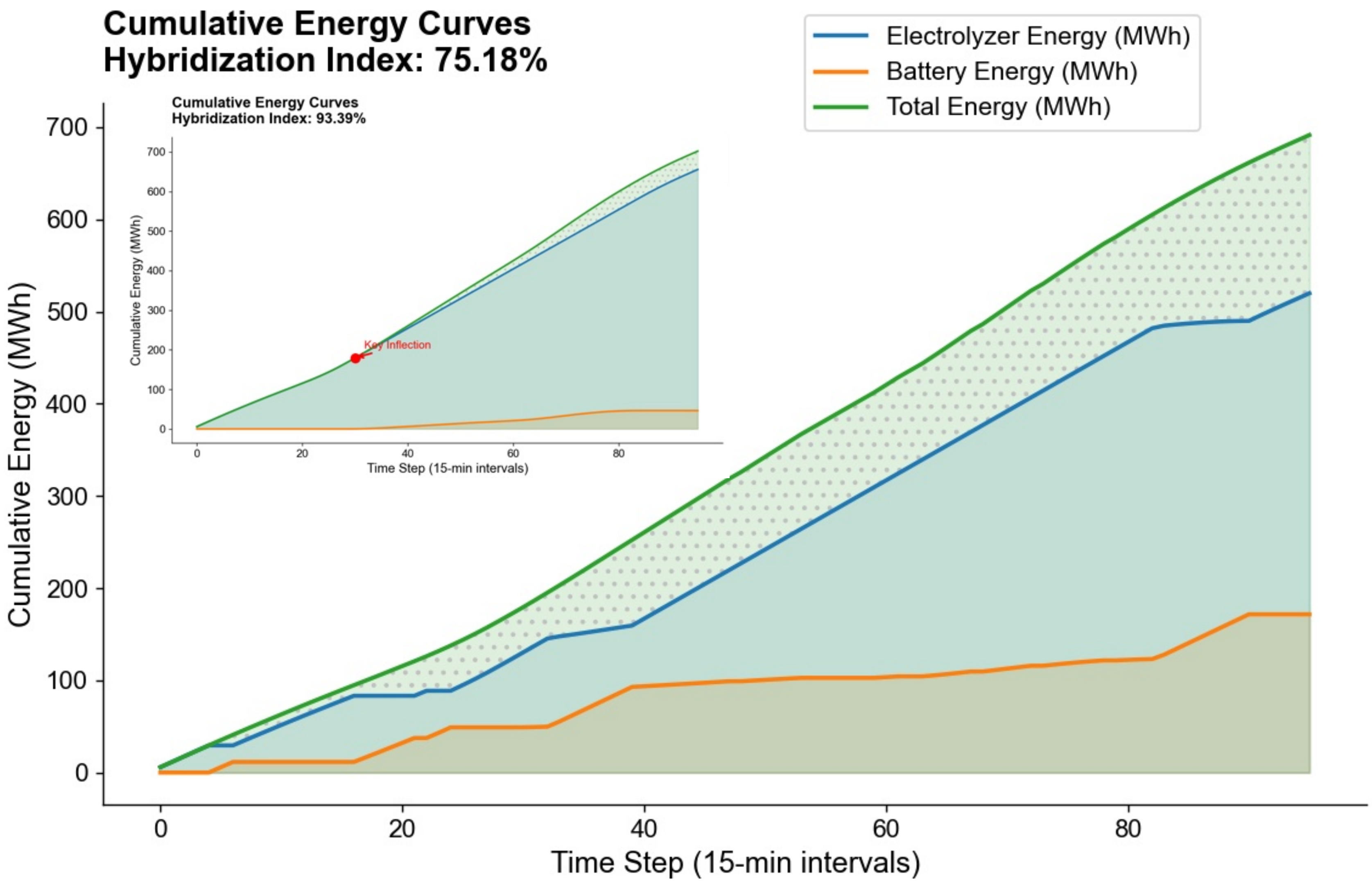
(b). Battery Discharging Profile



(c). Battery SOC Profile



(d). Electrolyser Power Profile



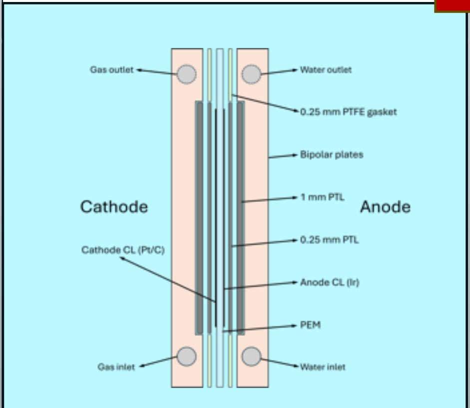
Hybridization Index

(H) = 93.39%

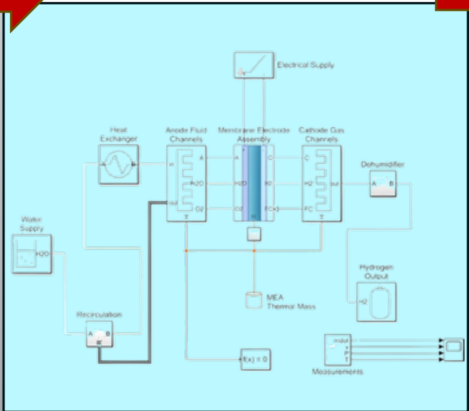
Hybridization Index

(H) = 75.18%

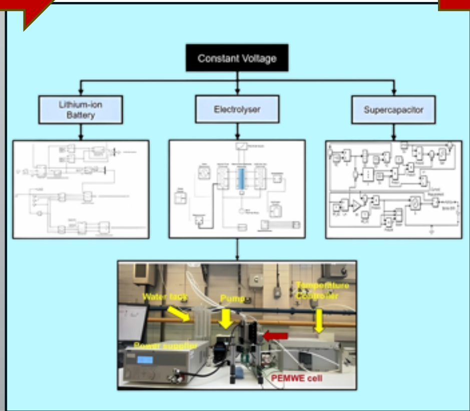
Experimental Setup



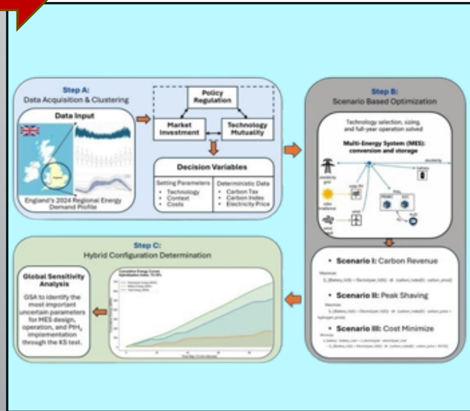
Electrode Simulation



HESS Process Modelling

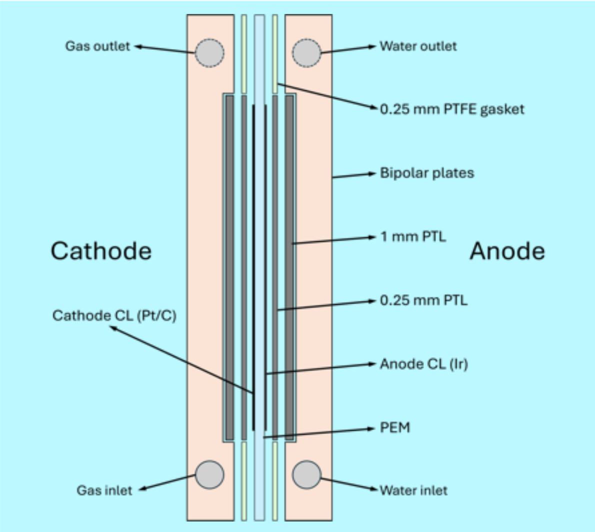


System Sizing



- Database Construction of Electrochemical Characterization, Parameterization & Visualization

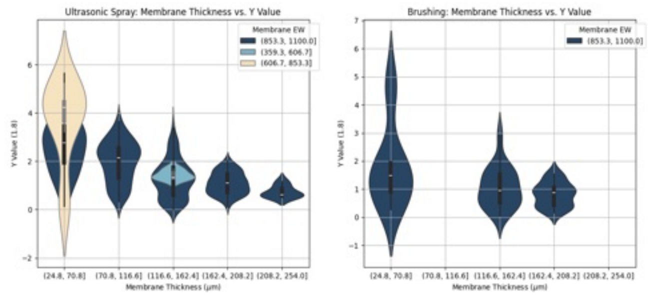
Physiochemical Parameterisation

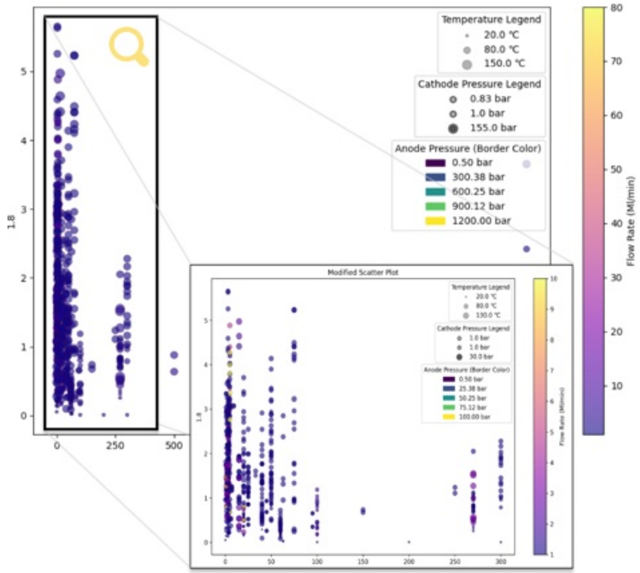


Eelectrode Parametrization

Abbreviation	Feature Name	Variable Range
OpTemp	Operating Temperature (°C)	20 to 130
OpPress	Operating Pressure (bar)	1 to 30
FlowRt	Flow Rate (ml/min)	0.1 to 2000
ActArea	Active Area (cm^2)	1 to 250
CCM/GDE	Catalyst Coated Membrane/Gas Diffusion Electrode	0 (CCM) / 1 (GDE)
IrWt	Ir wt. % (in anode catalyst)	0 to 100
RuWt	Ru wt. % (in anode catalyst)	0 to 83.55
CWt	C wt. % (in anode catalyst)	0 to 77.67
OWt	O wt. % (in anode catalyst)	0 to 33.62
PSSC	Pure Substance/Supported Catalyst	0 (Pure) / 1 (Supported)
ICRAn	Ionomer/Catalyst Mass Ratio in Anode	0 to 5
PtWt	Pt wt. % (in cathode catalyst)	0 to 100
ICRCath	Ionomer/Catalyst Mass Ratio in Cathode	0 to 26.04
APMLoad	Anode Precious Metal Loading (mg cm^{-2} Ir/Ru/Pt/Pd ...)	0 to 5
CPMLoad	Cathode Precious Metal Loading (mg cm^{-2} Pt/Pd ...)	0 to 88.46
MembThk	Membrane Thickness (μm)	25 to 254
EW	Equivalent Weight (EW)	206 to 1219
MinStabCD	Minimum Stability Current Density (mA cm^{-2})	0 to 10
MaxStabCD	Maximum Stability Current Density (mA cm^{-2})	0 to 10

Characterisation & Visualization

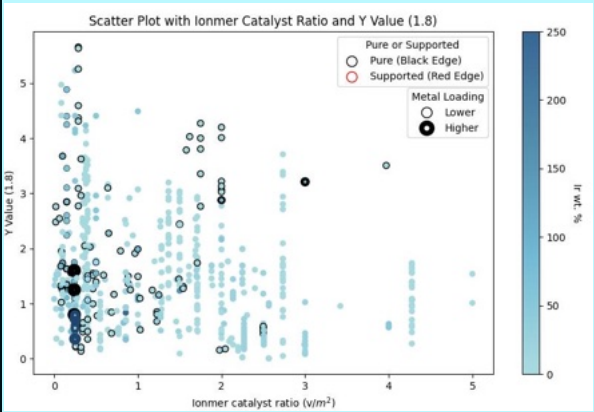




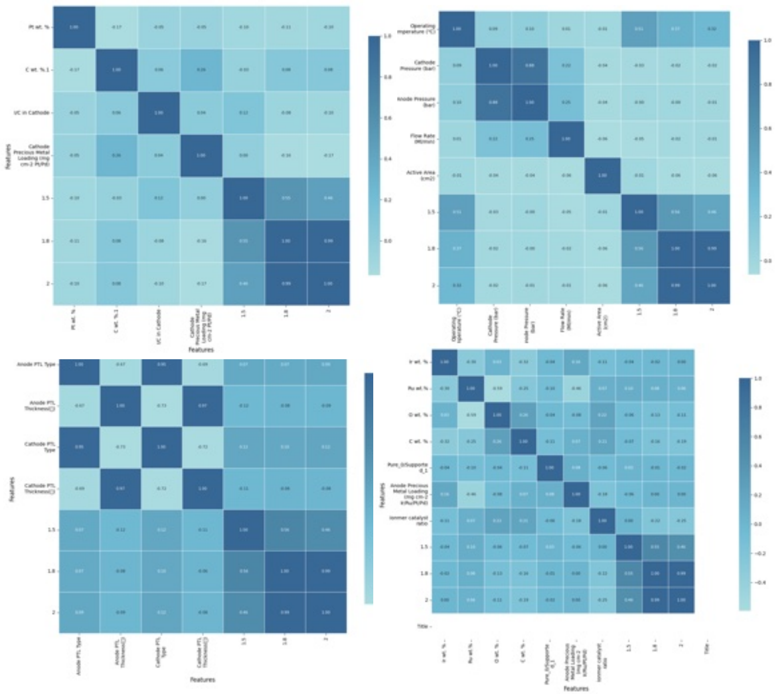
Augumentation Analysis

- Database Construction of Electrochemical Characterization, Parameterization & Visualization

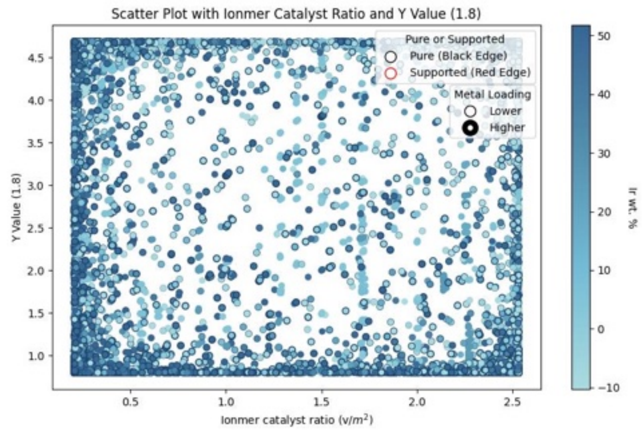
Descriptor Database

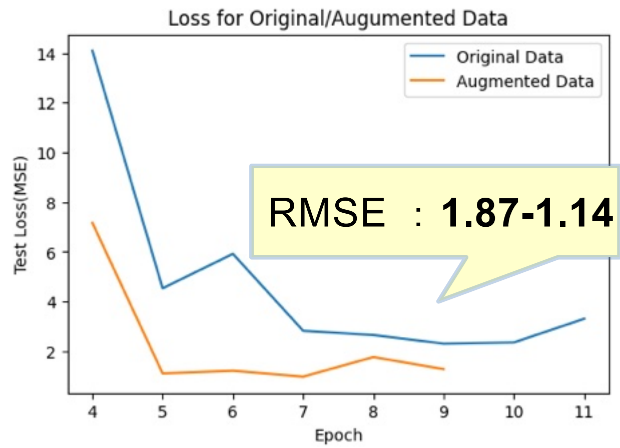


Correlation & Heatmap Analysis

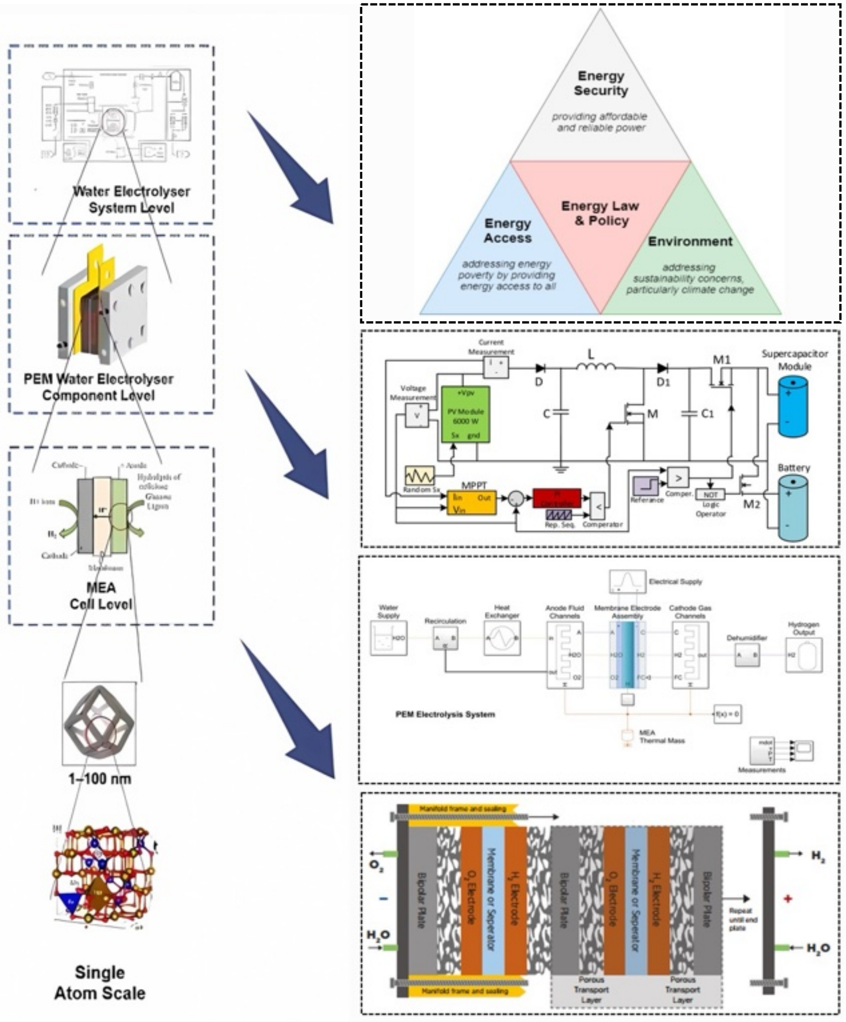


Augmentation





PEM-Integrated Hybrid Energy Storage Modelling and Optimization for Data Centre Resilience



Answer:

a). Nature of electrochemical process scaling, and how it influences energy system design?

b). How does **multiscale modelling** link cell-level physics with system-level assessment?

c). How is the **data-driven framework applied** to calibrate and evaluate electrochemical subsystems?

d). How are validated subsystem models integrated with **real-world** load and PV profiles in data centre simulations?

e). What does **resilience** mean in data centre energy systems-and how can HESS support it?

f). How does scenario-based optimization shape HESS sizing and control decisions?

Acknowledgement

- Dr Georgios Nikiforidis (⭐)
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- Prof Adham Hashibon
- Prof Natasha Khovanova
- Prof Xiaowei Zhang
- Prof Sai Gu
- Prof Shangfeng Du (⭐)
- Warwick Intelligent Energy System Group
- Birmingham Electrochemical Engineering Group
- Sustainable Energy Storage & Recycling Group

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