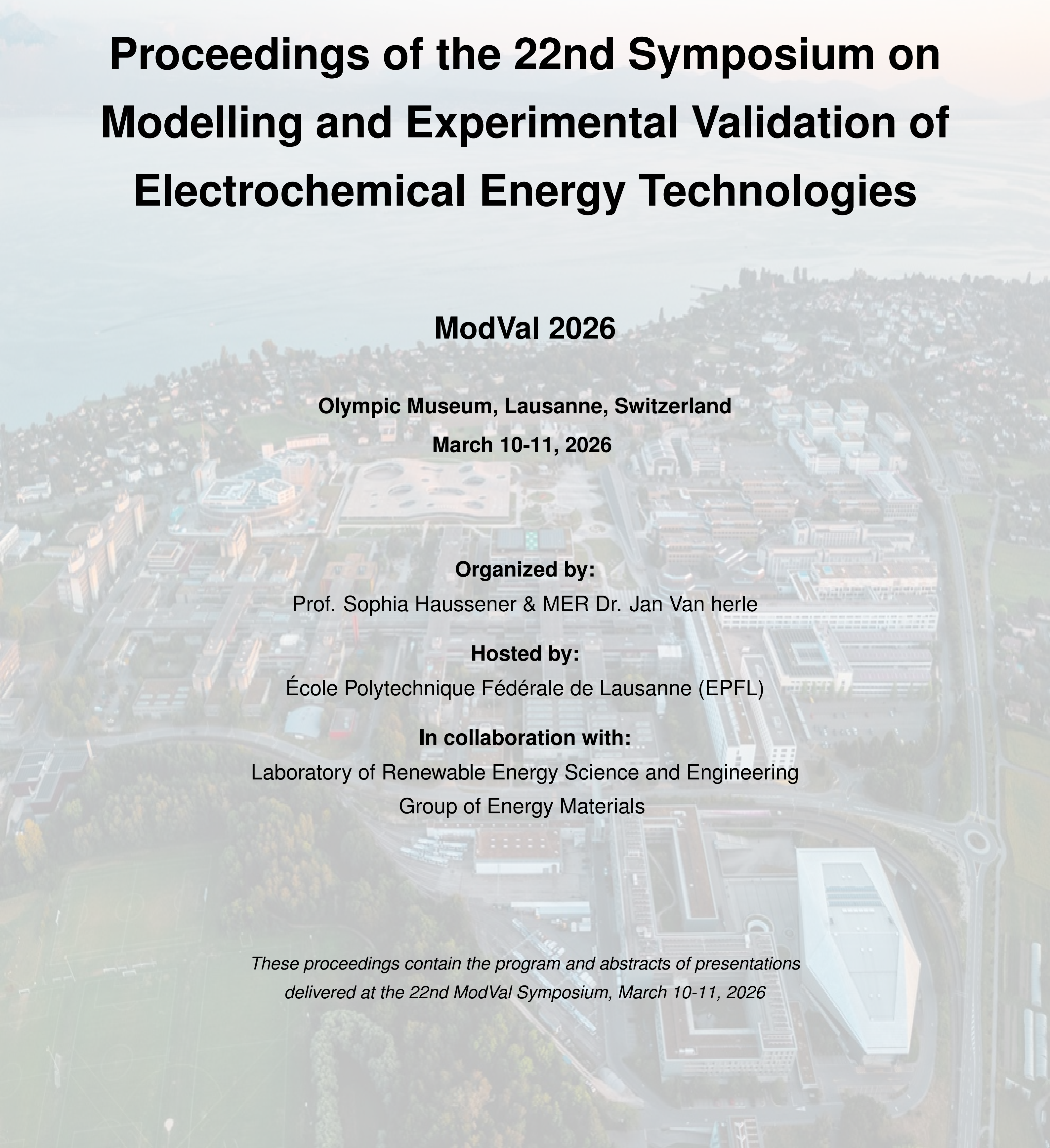

ModVal
2026
10–11 Mar, 2026
Lausanne, EPFL
Switzerland

Proceedings of the 22nd Symposium on Modelling and Experimental Validation of Electrochemical Energy Technologies

ModVal 2026

Olympic Museum, Lausanne, Switzerland
March 10-11, 2026

Organized by:
Prof. Sophia Haussener & MER Dr. Jan Van herle

Hosted by:
École Polytechnique Fédérale de Lausanne (EPFL)

In collaboration with:
Laboratory of Renewable Energy Science and Engineering
Group of Energy Materials

These proceedings contain the program and abstracts of presentations delivered at the 22nd ModVal Symposium, March 10-11, 2026

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Editors:

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22nd Symposium on Modeling and Experimental Validation of Electrochemical Energy Technologies (ModVal 2026)
Olympic Museum, Quai d'Ouchy 1, 1006 Lausanne, Switzerland, March 10-11, 2026

ModVal
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Program Overview

Tuesday March 10th		
07:30	Registration opens at entrance of the museum	
08:45	Welcome, Room: *Auditorium*	
09:00	**Plenary I, Room: *Auditorium***	
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10:00	Session A1: *Next Generation*	Session B1: *High temperature electrolysis*
11:00	Coffee Break@*Room Olympia*, Poster@*Room Olympia/Lausanne*	
11:30	Session A2: *Thermal impact*	Session B2: *High temperature fuel cells*
12:30	Lunch Break@Room Olympia, Poster@Room Olympia/Lausanne	
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13:10	Session A7: *Modelling II*	Session B7: *Transport in electrodes and membranes*
14:30	Closing remarks and announcement of **ModVal2027** at Room *Auditorium*	

Oral program

Each oral talk includes 17 minutes presentation and 3 minutes Q&A

	Tuesday March 10th	
07:30	Registration opens at entrance of the museum	
08:45	Welcome, Room: *Auditorium* (ground floor) Chair: **Sophia Haussener**, **Jan Van herle**	
09:00	Plenary I, Chair: **Sophia Haussener**, Room *Auditorium* (ground floor) **Curtis P. Berlinguette** (University of British Columbia) ***Reactive carbon capture***	
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	Session A: *Energy Storage* Room: *Auditorium* (ground floor)	**Session B: *Energy Conversion*** Room: *Coubertin* (2^{nd} floor)
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19:00	**Conference Dinner** at Olympic Museum	

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13:10	**Patricia Ogochukwu Mmeka** (Offenburg University of Applied Sciences)	**Christopher Arntsen** (SINTEF Industry)

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A307	**Manuel Landstorfer** (Weierstrass Institute for Applied Analysis and Stochastics) Modeling and simulation of porous electrodes with phase separation based on non-equilibrium thermodynamics and homogenization theory
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A503	**Sunil Kumar Rawat** (Imperial College London) Beyond Paris's Law: rethinking particle cracking, active material isolation, and degradation in lithium-ion cells by a mechanically coupled LAM model
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B310	**Nick Raue** (Fraunhofer Institute for Solar Energy Systems ISE) Implementation and validation of a PEMFC mesoporous substructure electrode model into a 3D CFD-Code
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B318	**Tancrède Oswald** (Friedrich-Alexander Universität Erlangen-Nürnberg) Model-Based Reduction of the Required Validity Space of Electrochemical Models for Efficient Testing
B319	**Kersten Schwab** (Karlsruhe Institute of Technology) Influence of the Cathode Catalyst Material Selection on the Cathode Gas Transport Processes in PEMFC
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B321	**Felix Benz** (Forschungszentrum Jülich) Microscopic Mechanical Models for PEM Compared to Real Cell Deformations
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B602	**Lourenço C. Vieira** (Zürcher Hochschule für Angewandte Wissenschaften) Studying Local Inhomogeneities in Zero-gap CO_2 Electrolysis via Validated 2D Multiphysics Simulation
B603	**Roberto Valenza** (École Polytechnique Fédérale de Lausanne) Hydrogen production by combined hydrothermal liquefaction and membraneless electrochemical reforming of organic waste with integrated CO_2 capture
B604	**Aviral Rajora** (TNO) Using simulations and machine learning for efficient electrochemical CO_2 reduction for ethylene production
B605	**Natalie Frassl** (École Polytechnique Fédérale de Lausanne) Investigating Morphological Evolution and Degradation of Electrocatalysts During Electrochemical CO_2 Reduction
B606	**Etienne Boutin** (École Polytechnique Fédérale de Lausanne) (Micro-)kinetic Effect on Selectivity during Pulsed Electrolysis: Exploring the Space of Electrochemical Parameters

B607	**Matthieu Dessiex** (École Polytechnique Fédérale de Lausanne) The Cathode Ionomer as an Interfacial Modulator in Electrolyte-Free CO_2 Electrolysis
	B7 Transport in electrodes and membranes, and diagnostics
B701	**Alessio D'Alessandro** (Ansaldo Green Tech) Insight on in-cell three-electrode EIS using an insulated endplate as pseudo-reference
B702	**J. Raphael Seidenberg** (RWTH Aachen University) Definition and Interpretation of Concentration and Activation Overpotentials
B703	**J. Raphael Seidenberg** (RWTH Aachen University) Modeling of electrochemical impedance spectroscopy measurements under gas evolution
B704	**Mostafa Delpisheh** (Newcastle University) Coupled electrochemical–MHD modeling of magnetic-field-induced water electrolysis in acidic electrolyte
B705	**Axel R. Dullak** (Zürcher Hochschule für Angewandte Wissenschaften) Local Lattice Boltzmann Implementation for Electrochemical Transport in OpenLB
B706	**Kira Ohlinger** (Friedrich-Alexander-Universität Erlangen-Nürnberg) Energy and Exergy Balancing in Modular Electrochemical and Fluid Dynamic Systems Modelling
B707	**Jürgen Fuhrmann** (Weierstrass Institute) Modeling and simulation of a closed electrochemical cell via an ion-conserving modified Poisson–Boltzmann model with dielectric decrement
	B8 Solar-driven electrochemsitry
B801	**Thomas Heipke** (École Polytechnique Fédérale de Lausanne) Investigation of a tandem membrane-photoelectrode assembly for solar hydrogen production
B802	**Simone Pokrant** (Paris-Lodron University of Salzburg) Current decay curves and degradation of oxynitride photoanodes for renewable hydrogen generation
B803	**Abhinav Bhanawat** (École Polytechnique Fédérale de Lausanne) Optimizing fiber geometry in transparent fibrous conducting substrates for enhanced photoelectrochemical performance
B804	**Paul Feurstein** (École Polytechnique Fédérale de Lausanne) Predicting Operation and Degradation of Photoanodes

Modval 2026 Plenary speakers

Prof. Alejandro A. Franco (Unviersité de Picardie Jules Verne)

Prof. Alejandro A. Franco is a Full Professor at the Université de Picardie Jules Verne, an Honorary Member of the Institut Universitaire de France and Affiliate Professor at University of Washington (Seattle, USA), with over 25 years dedicated to the multiscale modeling of electrochemical energy devices, and batteries in particular. His pioneering work, recognized by two ERC grants, integrates physics-based simulations, AI, and mixed reality to optimize battery manufacturing. He was honored with the 2019 French Prize for Pedagogy Innovation for his use of Virtual Reality in battery education, and is the recipient of the 2025 Battery Division Whittingham Mid-Career Award of the Electrochemical Society. Prof. Franco published more than 180 publications, 12 book chapters, 23 patents, and has delivered more than 230 invited lectures. He also coordinates the Erasmus+ i-MESC MSc. programme, at the crossroads between battery science, engineering and digitalization. He is the co-founder and CSO of Aikemics, a startup providing unique digital solutions for the battery industry.

Prof. Curtis P. Berlinguette (University of British Columbia)

Prof. Curtis P. Berlinguette leads an interdisciplinary team that designs and builds electrochemical reactors to accelerate decarbonization. Dr. Berlinguette is a Distinguished University Scholar at the University of British Columbia, where he is a Professor of Chemistry and Chemical & Biological Engineering. He is also a Fellow of the Royal Society of Canada, CIFAR Program Director, and Principal Investigator at the Stewart Blusson Quantum Matter Institute (SBQMI). His academic group has advanced a range of clean energy applications including CO2 utilization, membrane reactors for decarbonizing the chemicals industry, and lower-temperature fusion.

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Conference Venue

Olympic Museum
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Location: Le Musée Olympique, Quai d'Ouchy 1, 1006 Lausanne
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Oral Abstracts

Session A: Energy storage

An experimentally-validated modeling workflow coupling electrochemistry and solid mechanics on resolved microstructures of ASSB generated from manufacturing

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Abstract

In all-solid-state batteries (ASSBs), mechanical stress generated during the (de)lithiation of composite electrodes critically influences cell longevity due to its role in triggering degradation mechanisms. These stresses arise from local volume variations in the active materials, which are intrinsically linked to spatial lithium concentration gradients during cycling. In particular, the active material LiNixMnyCozO2 exhibits lithiation-dependent volume changes that must be considered to accurately capture stress evolution in ASSBs. In this work, we introduce a 3D mesoscale model that fully couples electrochemistry and solid mechanics by incorporating for lithium-concentration–dependent volumetric strain of the active material and its reciprocal effect through a stress-dependent chemo-mechanical potential governed by hydrostatic stress. The electrode microstructure used in this model is generated from wet manufacturing process simulations, including slurry preparation, drying, and compression [1]. Two compression techniques, uniaxial and warm isostatic, are applied to investigate the influence of each on cell performance and capacity fade.

Our computational workflow employs a continuum mechanics framework to resolve the mechano-electrochemical interactions within the composite cathode of an ASSB half-cell. The results reveal that total cell volume change is strongly dependent on both the C-rate and the applied stack pressure [2,3]. Additionally, we observe that mechanical effects and their interaction with electrochemical processes substantially impact the microstructural evolution of the electrode during cycling. The proposed modeling workflow is finally validated through experimental data.

Keywords: ASSBs, Full-coupling, Mechano-electrochemistry, Composite cathode, Volume change.

References:

[1] M. Alabdali, F. M. Zanotto, M. Duquesnoy, A.-K. Hatz, D. Ma, J. Auvergniot, V. Viallet, V. Seznec, A. A. Franco, *Journal of Power Sources* **2023**, *580*, 233427.
[2] S. Ben Hadj Ali, M. Alabdali, V. Viallet, V. Seznec, A. A. Franco, *Journal of Power Sources* **2025**, *630*, 236131.
[3] "S. Ben Hadj Ali, M. Alabdali, V. Viallet, V. Seznec, A. A. Franco, *Batteries & Supercaps* **2025**, *00*, e202500540.

Electrochemical Modeling of Silicon in Lithium-Ion Batteries Using a Multi-Species, Multi-Reaction Framework with Atomistic Insights

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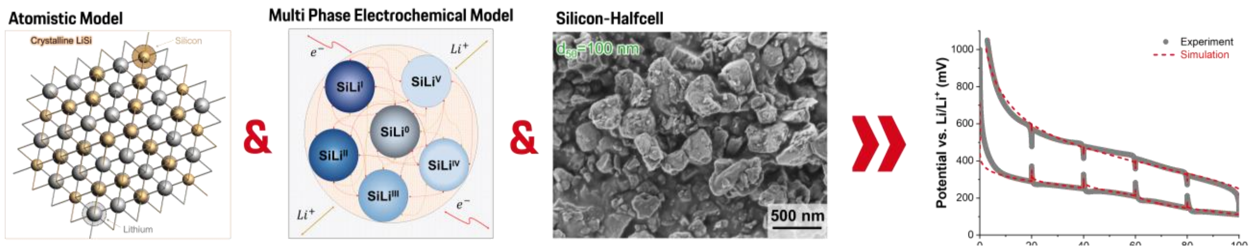
Abstract

Silicon is one of the most promising anode materials for next-generation lithium-ion batteries due to its exceptionally high theoretical capacity and potential to substantially increase cell-level energy density. However, Silicon electrodes exhibit complex electrochemical behavior characterized by pronounced voltage hysteresis, path-dependent equilibrium potentials, particle-size-dependent phase plateaus, and extended relaxation times, which originate from the multi-phase Li–Si alloy system and cannot be captured by conventional Doyle–Fuller–Newman (DFN) type models. Existing hysteresis approaches typically rely on empirical descriptions (e.g., Plett or Preisach-type descriptions) that do not provide mechanistic insight and fail to reproduce phase evolution.

In this work, we present a Multi-Species Multi-Reaction (MSMR) electrochemical model approach that explicitly resolves the phase transformations during (de)lithiation of Silicon. Each Li–Si phase is treated as a chemically distinct redox couple with respective equilibrium potential, derived from modified Nernst relations and parameterized using atomistic formation energies. The model incorporates asymmetric reaction pathways, phase-fraction evolution, and thermodynamic lithium redistribution during relaxation, consistent with experimental observations.

Model validation was performed using silicon half-cells cycled at C/40 under constant-current and pulse–relaxation conditions. The MSMR framework accurately reproduces key electrochemical features, including voltage hysteresis, lower-cutoff-potential-dependent open-circuit behavior, and long-time relaxation dynamics, with RMSE values of 25–50 mV. By mechanistically linking atomistic phase energetics to macroscopic electrode behavior, this approach offers a physically grounded pathway toward improved state estimation, advanced control strategies, and the rational design of Si/graphite composite anodes for next-generation high-energy lithium-ion cells.

Keywords: ModVal2026, Batteries, Silicon anodes, Voltage hysteresis, Multi-Species Multi-Reaction model



References:

N. Papadopoulos, O. Queisser, S. Arnold, S. D. Bhende, J. E. Mueller, S. Schwunk, V. Presser, Electrochemical Modeling of Silicon in Lithium-Ion Batteries Using a Multi-Species, Multi-Reaction Framework with Atomistic Insights, (submitted).

A Multiscale Numerical Investigation of LNMO/LFP Blended Cathodes

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Abstract

Blended cathodes combining different active materials have emerged as a promising strategy to exploit complementary electrochemical properties while mitigating the intrinsic limitations of individual components. In this context, cobalt-free systems based on lithium nickel manganese oxide (LNMO) and lithium iron phosphate (LFP) are particularly attractive, as they combine high operating voltage with enhanced safety and cycling stability. Inspired by the experimental study of Versaci et al. (2024), this work presents a 4D multiscale numerical investigation of LNMO/LFP blended cathodes aimed at elucidating the role of material architecture and LFP content on electrochemical performance. Unlike homogenized or effective-medium descriptions, LNMO and LFP are treated as physically and electrochemically distinct phases throughout the modelling framework.

At the particle scale, the strong mismatch in characteristic dimensions between the two materials is explicitly accounted for by modelling a micrometric LNMO particle (10 µm) partially covered by nanometric LFP particles ($\approx$200 nm). Separate transport and kinetic descriptions are retained for each phase, enabling the investigation of local lithium transport and potential lithium exchange between the two cathodic materials.

The analysis is subsequently extended to the electrode scale through simulations of lithium-ion battery half-cells. The cathode is represented as a packed bed of spherical LNMO particles acting as active cores, each surrounded by a homogeneous porous shell whose solid phase corresponds to LFP. This core–shell architecture preserves the separation between the two active materials and avoids homogenization into an equivalent blended phase, while enabling a systematic assessment of the effect of LFP content on the macroscopic electrochemical response.

Keywords: 4D model, Blended Cathodes, Lithium-ion Battery
Acknowledgement: This work was funded by the European Commission within the Horizon Europe research and innovation programme through the GA no 101137725 (BatCat).

References: Versaci, Daniele, et al. "Tailoring cathode materials: A comprehensive study on LNMO/LFP blending for next generation lithium-ion batteries." *Journal of Power Sources* 613 (2024): 234955.

Development and validation of a temperature and heat flux sensor for lithium-ion battery thermal characterization

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Abstract

Accurate characterization of local heat fluxes on battery surfaces is essential for the development of reliable thermal management and diagnostic systems. This work presents the design, modeling, and steady-state calibration of a temperature and heat flux sensor (THFS) based on commercial thermoelectric modules (TEMs). The sensor is designed to enable simultaneous measurement of temperature and heat flux while preserving flexibility for active boundary-condition control. A steady-state heat flow meter (HFM) calibration setup, adapted from the methodology proposed by Rizzo et al., is employed to establish a traceable relationship between the thermoelectric voltage output and the applied heat flux. Based on this calibration, effective thermoelectric parameters of the THFS assembly, including an effective Seebeck response, thermal conductivity, and sensor sensitivity, are derived over a temperature range from $-5℃ \text{ to } 60℃$. The resulting calibration yields a temperature-dependent sensor sensitivity of $G(T) = 141\mu Vm^2W^{-1} + 0.61\mu Vm^2W^{-1}K^{-1} \times T$ and a maximum effective Seebeck response of $51.3 \pm 3.5\, mVK^{-1}$ under steady-state heating conditions. Reproducibility tests conducted on two identically fabricated THFS units demonstrate deviations below 3% in voltage output and 14% in heat flux, confirming the robustness of the calibration procedure. A coupled thermal-electrical digital-twin model reproduces the experimentally obtained calibration data with a maximum deviation below 6%, supporting the validity of the simplified modeling approach. Parametric simulation studies investigating insulation thickness and thermal adapter block (TAB) geometry indicate an optimal configuration featuring a $5\ mm$ insulation layer and a $36\ mm$ truncated-pyramid TAB, promoting quasi-one-dimensional heat transfer.

The combined experimental numerical framework provides a traceable and reproducible methodology for boundary-condition design in battery thermal management. The developed THFS demonstrates compactness and adaptability for localized heat-flux sensing on cylindrical $LiFePO_4$ cells and may be extended to other electrochemical or thermally active systems following further refinement of the temperature attribution within the thermoelectric assembly.

Keywords: ModVal2026, heat flux sensing, thermoelectric calibration, battery thermal management, THFS

Fitting thermal parameters from electrical data gives lumped models of heterogeneous cells, by predicting their effective temperature

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Abstract

Temperature impacts the performance of all electrochemical systems. A battery forms a temperature gradient when it is used, which in turn drives spatial variations in the electrochemical behaviours. Lumped models are desirable for battery management and pack design applications, but volume-averaging away any spatial effects leads to incorrect results, due to the thermal-electrochemical coupling. Spatial models can be used instead, however they are too computationally expensive for use in design optimisation, or for online battery management and control. This motivates the problem of how best to approximate heterogeneous cell behaviour, using only simple lumped models. We develop a novel modelling and experimental framework to address this gap. Our models capture the emergent behaviours of heterogeneous battery systems, whilst being computationally light enough for use in management and optimisation problems. A cell or battery with a temperature gradient will still show some overall impedance; lightweight models can therefore be created if the heterogeneous impedance can be predicted. We demonstrate how to do this, by first defining the 'effective temperature' of a cell, and then building simple models and experiments to identify it. Effective temperature is a rigorous alternative to volume-averaging, and gives a single number which captures the intricate couplings between temperature, charge density, and current density on cell impedance. Since electrical performance depends on cell temperature, cell temperature can be inferred from electrical performance. We exploit this to develop our experimental protocols, which build effective temperature models using only readily available battery testing equipment. Effective temperature cannot be directly measured, so the experiments are carefully designed using cell impedance mapping, pack instrumentation, and thorough thermal control, which allows for an in-depth validation of the method. The results give a framework for accurate electrical-thermal modelling, which remains accurate when faced with real-world heterogeneity, and does not require complex or expensive thermal experiments. Furthermore, the resulting models are computationally lightweight, making them immediately valuable for pack design, thermal management selection, and battery management applications.

Keywords: heterogeneity, thermal modelling, parameter identification, reduced-order models

Degradation and Reformation of the Solid Electrolyte Interphase at the Onset of Thermal Runaway

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In Li-ion batteries, the exothermic decomposition of the solid electrolyte interphase (SEI) near 60 °C initiates a self-heating phase at the onset of thermal runaway [1]. The resulting heat accumulation raises the cell temperature until kinetically hindered cathode oxidation reactions become activated above ~200 °C, triggering thermal runaway [2]. The SEI is a layer that forms at the negative electrode surface and suppresses electrolyte reduction, thereby limiting initial gas evolution and enabling stable battery operation. Its structure depends on formation conditions and electrolyte composition [3], with layered and mosaic configurations, shown in Figure 1, being reported as relevant morphologies [4]. Identifying thermally stable SEI structures is therefore essential for improving thermal resilience through controlled formation.

In this work, we adapt a kinetic Monte Carlo (kMC) model [5] to reveal the decomposition and reformation of the SEI under thermal stress. The temperature dependence of the reaction kinetics and transport was developed based on prior experimental [6] and theoretical work and adapted for kMC modelling input. The thermal degradation of multiple layered and mosaic type SEI structures is studied in order to develop structure-property relationships to correlate initial configuration to the thermal stability of the SEI.

The results reveal that the conductive salt $LiPF_6$ is hydrolysed by water impurities at the surface of the SEI, forming solid SEI species and HF. The HF then reacts with exposed LiEDC and Li_2CO_3, decomposing these species and forming LiF at the SEI surface. LiEDC and Li_2CO_3 formed from EC are predominantly located at the SEI surface. The distribution of LiEDC close to the surface is critical because its larger molecular size leads to a greater exposed surface area when decomposed, enhancing repeated decomposition and reformation. This highlights the strong coupling between SEI composition, spatial distribution, and dynamic degradation processes, and provides guidance for controlling formation conditions toward more thermally stable SEI structures.

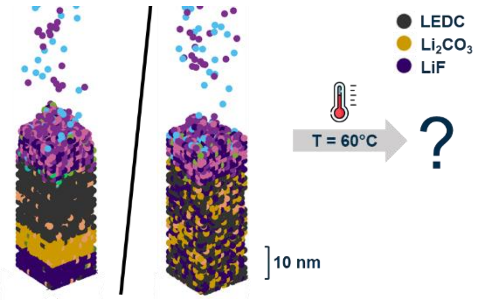

Figure 1: Left: Layer type, right: Mosaic type SEI

References:
[1] F. Baakes, M. Lüthe, M. Gerasimov, V. Laue, F. Röder, P. B. Balbuena, and U. Krewer, J. Power Sources 522, 230881 (2022).
[2] X. Feng, M. Ouyang, X. Liu, L. Lu, Y. Xia, and X. He, Energy Storage Mater. 10, 246 (2018).
[3] F. Schomburg, B. Heidrich, S. Wennemar, R. Drees, T. Roth, M. Kurrat, H. Heimes, A. Jossen, M. Winter, J. Y. Cheong, and F. Röder, Energy Environ. Sci. 17, 2686 (2024).
[4] H. Adenusi, G. A. Chass, S. Passerini, K. V. Tian, and G. Chen, Adv. Energy Mater. 13, 2203307 (2023).
[5] K. Hankins, M. H. Putra, J. Wagner-Henke, A. Groß, and U. Krewer, Adv. Energy Mater. 2401153 (2024).
[6] L. Schmidt, K. Hankins, L. Bläubaum, M. Gerasimov, and U. Krewer, Chem. Sci. 10.1039.D4SC08105F (2025).

Keywords: solid electrolyte interphase, thermal runaway, degradation

Quantifying the impact of secondary particle cracks on High-Nickel insertion batteries

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Abstract

While transition metal oxide electrodes with high nickel content provide a high volumetric and specific capacity, they also show accelerated degradation, in the form of changes to the crystalline structure, surface passivation accompanied by electrolyte decomposition and mechanical degradation due to cracking [1,2].

Quantifying and identifying dominant degradation mechanism remains challenging. Established in-operando methods cannot distinguish between contributions from these degradation mechanisms, resulting in lumped properties, influenced by both chemical and morphological degradation.

This work presents a workflow which aims to quantify the impact of secondary particle cracks on electrode performance and isolate it from other degradation mechanisms.

In order to do so, a two-pronged approach is used. Cathodes in various aging states (Up to 500 cycles, 1 - 5C) are characterized in regards to the evolution of their lumped properties, using established electrochemical methods. This includes capacity, resistance and the apparent diffusion coefficient. In parallel, focused ion beam tomography was conducted to acquire high-resolution 3D datasets of the electrodes. The datasets are then processed applying a multi-stage analysis pipeline, which includes 3D U-Net models, to extract several geometrical descriptors that are associated with morphological properties of NMC particles [3]. These serve as input for virtual characterization experiments using a state-of-degradation model [4], to determine the effect of the morphological changes, independent of other degradation processes. Lastly, by subtracting the influence of the morphology from the experimentally observed cathode characteristics, deeper insight into the evolution of the remaining degradation processes is obtained.

Source:
[1] D.P. Abraham et al., Electrochemistry Communications, 2002, **4**, 620-625
[2] W.M. Dose et al., ACS Appl. Mater. Interfaces, 2022,**14**, 13206-13222
[3] P. Rieder et al., npj Comput. Mater., 2025, **11**, 232
[4] M. Fath et al., J. Electrochem. Soc, 2026, **173**, 010511

Keywords: high-nickel cathodes, imaging, degradation analysis, battery modeling

Increased effective diffusion coefficient of secondary particles due to beneficial effects of cracking

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Abstract

While cracking contributes to degradation in battery cathodes, it also allows liquid electrolyte to infiltrate secondary particles of the cathode active material [1]. Consequently, the particle's surface area grows and its diffusion path decreases [1]. This effect has been shown to increase the effective diffusion coefficient by over one order of magnitude [1]. As battery models rely on an accurate diffusion coefficient, further investigation is essential.

Herein, this study analyses fully resolved spherical agglomerates in a 3D framework with a diameter of 10 µm (Fig. 1a). Using the multiphase-field method and building on previous work of our group [2,3], anisotropic chemo-mechanical strain and resulting microcrack formation are modelled (Fig. 1b). We compare the effective diffusion coefficients of cracked and uncracked secondary particles via potentiostatic intermittent titration technique (PITT) simulations (Fig. 1c). This study is the first analysing how 3D microcracking increases the effective diffusion coefficient, supporting the refinement of battery models.

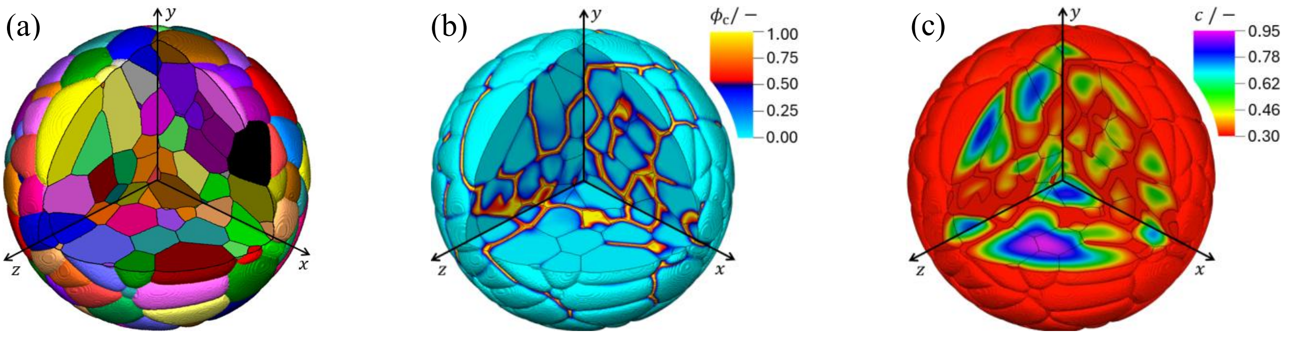

Figure 1: Secondary particle morphology of NMC with colors marking primary particles (a), crack order-parameter ϕ_c (b) and Li-ion concentration c after electrolyte infiltration (c).

References:
1. Trevisanello et al., Polycrystalline and Single Crystalline NMC Cathode Materials – Quantifying Particle Cracking, Active Surface Area, and Lithium Diffusion, *Advanced Energy Materials*, 11, 2003400, 5 2021.
2. Daubner et al., Modeling anisotropic transport in polycrystalline battery materials, *Batteries*, 9(6):310, 2023.
3. Schöller et al., Phase-field modeling of crack propagation in heterogeneous materials with multiple crack order parameters, *Computer Methods in Applied Mechanics and Engineering*, 395:114965, 5 2022.

Keywords: effective diffusion coefficient - microcracking - NMC - multiphase-field method

A Physics-Informed Model for Chemo-Mechanical Damage in Lithium-Ion Battery Particles

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Abstract

The durability and performance of lithium-ion batteries are affected by microscale processes within active material particles. During lithiation and delithiation, lithium diffusion leads to concentration gradients that cause volumetric expansion and contraction, resulting in internal stresses. Over repeated cycling, these chemo-mechanical effects can promote fatigue and fracture, contributing to particle degradation. Due to the small length scales and coupling of the underlying mechanisms, experimental analysis of these processes remains challenging.

This work presents a unified theoretical and computational framework for modeling chemical diffusion, mechanical stress, and damage evolution at the single-particle level. A one-dimensional, spherically symmetric NMC622 cathode particle is considered, where each process is governed by a differential equation. Lithium diffusion determines the concentration distribution, mechanical equilibrium defines displacement and stress fields, and material degradation is captured using a phase-field-like damage formulation. The damage variable provides a continuous description of material integrity and introduces feedback on both diffusion and mechanical response.

The resulting system of coupled, nonlinear equations is solved using Physics-Informed Neural Networks (PINNs). By incorporating the governing equations together with boundary and initial conditions into the training process, PINNs yield physically consistent and smooth solutions while maintaining computational efficiency.

The proposed framework serves as a modeling tool for investigating intercalation-induced stresses and particle-level damage in lithium-ion battery materials and provides a basis for further studies on degradation mechanisms at the microscale.

Keywords: PINN, single-particle model, mechanics, damage

Machine Learning Model–Based Electrochemical Diagnostics for Comprehensive Lithium-Ion Battery Health Assessment

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Lithium-ion batteries (LIBs) represent the enabling technology for electric mobility. Currently, understanding the State of Health (SoH) of a lithium-ion battery is primarily based on predicting capacity retention, which provides limited information on the type of degradation occurring inside the cell. Beyond capacity retention, Loss of Lithium Inventory (LLI) and Loss of Active Material (LAM) are two quantities that can be extracted from charge–discharge curves to gain additional insights into degradation mechanisms. Previous studies have related LLI to the loss of cyclable lithium (causing capacity fade), and LAM to portions of electrode material that become electrochemically inactive (causing both capacity fade and power loss). Quantifying degradation in terms of LLI and LAM can therefore provide more detailed diagnostic insight into battery ageing and support the development of strategies to address the underlying degradation mechanisms separately. However, the estimation of these parameters is typically achieved through physics-based electrochemical models, such as pseudo-two-dimensional (P2D) frameworks, or through dedicated post-processing of experimental data, both of which rely on time-consuming and computationally demanding procedures. As a result, the direct quantification of LLI and LAM remains challenging for practical, in-operando applications. In this context, data-driven approaches based on machine learning models offer a promising alternative to enable fast, scalable, and in-operando estimation of LLI and LAM for battery health diagnostics in electric vehicle applications. In this work, we present recent results on the data-driven prediction of capacity retention, Loss of Lithium Inventory, and Loss of Active Material in Nickel Manganese Cobalt (NMC) lithium-ion batteries using in-operando measurements. The study is based on an experimental database of NMC cells aged under laboratory-controlled conditions, designed to reproduce realistic driving scenarios through different combinations of temperature, state-of-charge window, and current rate. The dataset includes electrochemical impedance spectra, charge/discharge data, and temperature measurements acquired during cycling, which are jointly provided as inputs to the proposed framework. The prediction of capacity retention, LLI, and LAM is performed with an attention-based neural network model built on Transformer encoders (multi-head self-attention with positional encoding) that map each input sequence into a fixed-dimensional latent representation via padding-aware pooling. The learned representations are further conditioned on the operating conditions and used to estimate the different battery health indicators, enabling the model to capture complex and non-linear relationships between in-operando measurements and the underlying degradation processes. The proposed approach achieves accurate predictions for all health indicators, with a mean absolute error below 0.02 across the full ageing range, a level of accuracy that is challenging to attain with alternative modelling approaches when relying on a comparable amount of experimental data. An analysis of the learned attention weights provides insight into the relative importance of the different input features and shows that electrochemical impedance information plays a dominant role in the prediction of capacity retention, LLI, and LAM. In particular, the attention maps highlight specific frequency regions of the impedance spectra as the most relevant contributors across different ageing conditions. These findings suggest that attention-based data-driven models can support advanced in-operando battery health diagnostics, with potential implications for practical monitoring and management of lithium-ion batteries.

Keywords: ModVal2026, Li-ion Battery, Machine Learning, Degradation

Monitoring Heterogeneous Deformation in Lithium Batteries Using Strain Gauges and Digital Volume Correlation

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Abstract

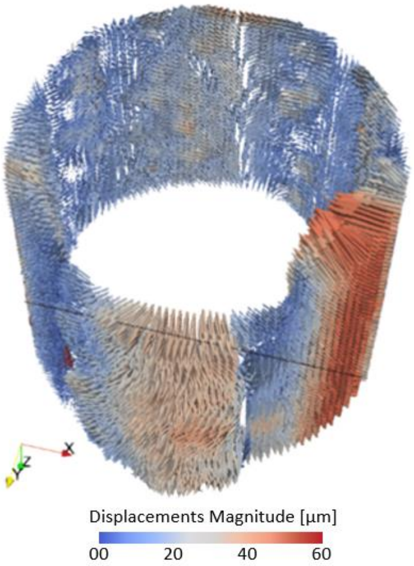

Figure 1: 3D in situ DVC displacement fields (amplified ×50) at the center of an 18650-cell casing between 0% and 100% SoC (real values in colormap)

The mechanical integrity of 18650 lithium-ion batteries (LIBs) is critical for ensuring their long-term performance and safety, particularly under repeated charge-discharge cycles. In this work, we present an innovative approach that combines operando measurements using strain gauge rectangular rosettes and *in situ* X-ray computed tomography imaging with Digital Volume Correlation (DVC) to investigate the spatially heterogeneous mechanical behavior of cylindrical cells. Four strain gauge rosettes, strategically placed around the cell casing, provide localized measurements of circumferential, axial, and 45° strains, coupled with 3D displacement fields derived from DVC, reveal the global deformation patterns. Our findings demonstrate significant mechanical heterogeneities, with Von Mises stress value ranging from 50 to 125 MPa, closely tied to the jelly-roll winding architecture and electrode lithiation. Figure 1 illustrates the 3D displacement fields of the cell's casing from 0% to 100% State of Charge (SoC), highlighting heterogeneous deformation with localized displacement up to 60 µm. The observed heterogeneity in strain is highly repeatable across multiple charge–discharge cycles, as confirmed by the strain gauges measurements, indicating a reversible elastic response primarily governed by circumferential expansion. By correlating these local strain measurements with global 3D displacement fields obtained via DVC, this study provides a comprehensive view of electro-chemo-mechanical coupling in LIBs. Beyond improving understanding of mechanical degradation, this approach lays the groundwork for early fault detection in Battery Management Systems (BMS). Future perspectives should focus on integrating these mechanical insights with electrochemical and thermal BMS models to predict degradation pathways and optimize cell architecture, especially since other results from this study demonstrate that these mechanical deformations are correlated with electrochemical responses, notably through Incremental Capacity Analysis (ICA).

Keywords: Lithium-ion batteries, strain gauge rectangular rosette, von Mises stress; computed tomography; digital volume correlation.

Multisine electrochemical impedance spectroscopy

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Abstract

Electrochemical impedance spectroscopy (EIS) is a powerful tool for non-invasive battery characterisation. It provides a compact yet informative representation of the underlying physical processes across a broad range of time scales which can be used for applications ranging from temperature estimation to ageing diagnostics [1]. Traditionally, EIS employs sequential single-sine excitations, which restrict measurements to steady-state conditions (resting after long relaxation). In contrast, multisine excitation—a sum of sinusoids—significantly reduces measurement time and enables characterisation under operating conditions such as charging, discharging, relaxation, or temperature variations [2].

Despite its advantages, the implementation of multisine EIS remains limited, mainly due to bandwidth constraints and restricted data access in commercial potentiostats. In this work, we present a flexible multisine EIS setup using a commercial Battery Dynamics potentiostat, providing direct access to time-domain current and voltage data and exciting frequencies between 20 mHz and 1 kHz. We validate the setup by comparing multisine and single-sine impedance spectra, discussing the trade-offs of the two techniques and the verification of linearity and stationarity. Finally, we demonstrate multisine impedance measurements on a commercial Li-ion cell under diverse practical operating conditions, delivering a dataset for battery characterisation. We show how impedance can be measured during charging and discharging, and study how impedance not only depends on C-rate, but also on the direction of the current. This provides additional information for model parametrisation.

We emphasise that multisine EIS is particularly advantageous for performing rapid measurements over selected frequency bands under non–steady-state conditions (where single-sine EIS may fail). Moreover, we stress that potentiostat manufacturers should provide access to the raw current and voltage data, as this enables users to assess linearity and stationarity, estimate uncertainty bounds, and determine time-varying impedance.

[1] Hallemans, N., Courtier, N.E., Please, C.P., Planden, B., Dhoot, R., Timms, R., Chapman, S.J., Howey, D. and Duncan, S.R., 2025. Physics-based battery model parametrisation from impedance data. Journal of The Electrochemical Society, 172(6), p.060507.
[2] Hallemans, N., Howey, D., Battistel, A., Saniee, N.F., Scarpioni, F., Wouters, B., La Mantia, F., Hubin, A., Widanage, W.D. and Lataire, J., 2023. Electrochemical impedance spectroscopy beyond linearity and stationarity—A critical review. Electrochimica Acta, 466, p.142939.

Keywords: EIS, linearity, stationarity, operando, commercial potentiostat

Battery Health Monitoring and Degradation Analysis for EV Fleets: A Data-Driven Pipeline Approach

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Abstract

Battery aging diagnostics and state of health estimation are essential for extending lifetime, optimizing usage, and enabling second-life applications for EV batteries. We introduce the Battery Statistical DataFrame (Battery SDF), a compact and interpretable representation of real-world operational battery data. The Battery SDF encodes key stress factors including charge/discharge patterns, current load and temperature exposure into histogram-based features. These features can be derived from time series data or directly extracted from the battery management system, supporting both the use of existing historical data via post-processing or applications with minimal storage and processing requirements. The Battery SDF is particularly useful for standardizing battery data collection and processing protocols across multiple sources, supporting transfer learning and robust predictive data driven models. Its features are highly interpretable and enable actionable insights by comparing observed feature distributions to optimal reference distributions. Alone, the SDF performs strongly in state-of-health (SoH) and remaining useful life (RUL) prediction tasks, and the predictive power of our approach can be further enhanced by adding incremental capacity (dQ/dV) features, widely used in the literature to reveal electrode-specific degradation mechanisms.

Validation on open-source datasets demonstrates improved predictive accuracy while remaining interpretable, supporting actionable insights, multi-vendor analytics, battery passports, and field monitoring applications.

Keywords: Battery aging; State of health; Remaining useful life; Statistical data representation; Incremental capacity analysis; Battery management

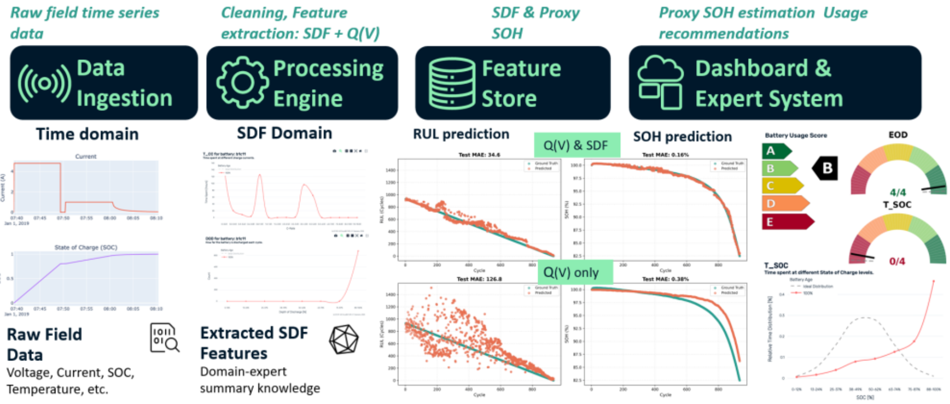

Figure 1. Overview of the data pipeline transforming raw battery measurements into insights displayed in the Battery Expert dashboard

3D Resolved Computational Modeling to Simulate the Electrolyte Wetting of a Lithium-Ion Battery Cell with 18650 Format

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Abstract

Electrolyte wetting is one of the most critical and time-consuming manufacturing process steps for lithium-ion batteries (LIB). Efforts to optimize wetting have motivated extensive experimental and computational studies. However, existing 1D and 2D models based on Lattice Boltzmann Method and Computational Fluid Dynamics methods are limited in their ability to capture the full complexity of the process. Although advanced 3D models provide deeper insight, their high computational cost restricts their applicability at the full-cell scale, particularly for heterogeneous cylindrical cells. To address this challenge, we present a novel macroscopic modeling approach capable of analyzing how macroscale heterogeneities influence electrolyte wetting in practical LIB geometries. Electrolyte wetting is investigated using parameters representative of an NMC111-graphite lithium-ion battery cell. A hierarchical strategy is adopted, beginning with a reduced-order 2D model and progressing to a full-scale 3D model that represents the complete spiral geometry of the cell. A pressure saturation formulation is derived and solved numerically using the finite element method to track the evolution of phase pressures and saturations during wetting. Results from the full-scale 3D model show that wetting is primarily driven by the jelly-roll architecture and capillary pressure. After 2 h of simulated wetting at an electrolyte inlet pressure of 800 kPa and an entry capillary pressure of 40 kPa, electrolyte saturation in a 3D 18650 cell reaches a plateau of 86%. At this stage, saturation is largely homogeneous throughout the cell, except near the outer fringes where gas entrapment occurs. The model enables unprecedented visualization of wetting in the inner windings of the jelly roll, offering insights that are difficult to obtain experimentally. Overall, this work advances the understanding of electrolyte wetting in LIB manufacturing and provides valuable guidance for optimizing wetting in cylindrical cell formats.

References:
[1] J. Wanner, M. Burgard, N. Othman, S. Singh, K. P. Birke, *Batteries & Supercaps* 2024, *8*, DOI 10.1002/batt.202400531.

[2] E. Yerumoh, I. Cardenas-Sierra, F. Fernandez, A. A. Franco, *Batteries & Supercaps* 2025, *8*, DOI 10.1002/batt.202500434.

Keywords: ModVal2026 (lithium-Ion batteries, electrolyte wetting, Jelly roll)

DEM-Based NCM622 Cathode Microstructures: Influence of Carbon-Binder-Domain Addition Method on Electrochemical Properties

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Abstract

The microstructure of lithium-ion battery electrodes determines their electrochemical performance and is strongly influenced by processing parameters. We present a virtual workflow that couples Discrete Element Method-based calendering simulation, microstructure reconstruction and electrode analysis to link cathode processing to structural properties. After validating this digital twin against a real cathode, we show the potential of our virtual work-flow by conducting electrochemical simulations.

The Discrete Element Method-based calendering model using virtual Carbon Binder Domain (CBD) bonds proves to represent the calendering process accurately, as deviations between experimental and simulated compaction stresses, as well as densities are less than 1.0% and 3.5%, respectively. As a next step, we reintegrate the electrochemically inactive material, i.e. the CBD, into the compressed particle pack using five reconstruction schemes. For each reconstructed microstructure, we compute pore size distributions, tortuosities, effective diffusivities, and electronic conductivities, and compare the results to experiments. The CBD addition method that combines surface roughening of the active material with a realistic binder gradient along the height of the electrode best reproduces experimentally measured transport properties. Therefore, our study recommends this representation method for most realistic microstructure recreation.

To show the potential of our experimentally validated digital twin for the cathode microstructure, we conduct electrochemical simulations across a range of C-rates. These predict capacities that align well with literature reports, with discrepancies not exceeding 3.2%, showing that our model can be used as the basis to detect diffusion-limiting C-rates. Overpotential analysis confirms that in this cathode Li-ion transport, rather than electronic conduction, is the primary bottleneck. This suggests that microstructure optimization in terms of improving ionic pathways is necessary for improving this electrode's performance. Our developed digital twin links electrode production process, structure and performance, providing a model that is able to assess limiting factors for battery performance and enables designing electrodes with targeted structural parameters to obtain desired performance.

Keywords: ModVal2026, Battery, DEM, Calendering, Microstructure, Conductivity

Microstructure-aware DFN models and the tortuosity of graded electrodes

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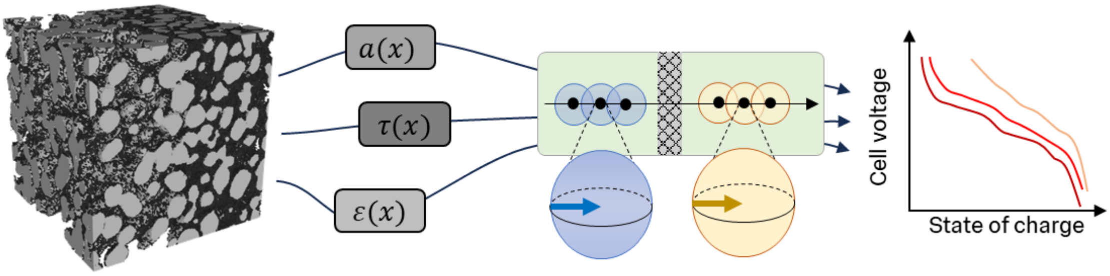
Abstract

Microstructure design of battery electrodes is critical for fast charging and high capacity in next-generation lithium- and sodium-ion cells. Porous-electrode (Doyle–Fuller–Newman-type) models capture the coupled transport-reaction physics but usually treat the electrode as a homogenized medium and fold microstructure into fitted, scalar “effective” parameters (e.g., Bruggeman-type tortuosity). While adequate for uniform electrodes, this breaks down for graded porosity, binder migration, bimodal particle distributions, or multilayer designs, where transport resistance is heterogeneous.

We introduce an efficient workflow that bridges 3D image-based electrode simulations and microstructure-aware cell-scale modelling using volume-averaged descriptors. We compute spatially resolved tortuosity factors τ(x), spatial porosity ε(x), and specific surface area a(x) and incorporate these closures directly into DFN-type cell models. This replaces *ad-hoc* global transport factors with physically interpretable, architecture-dependent descriptors capable of representing graded and bilayer electrodes. We further show that common characterization and parameter-identification workflows implicitly assume homogeneity and can therefore misattribute microstructure-driven limitations to material kinetics in structured electrodes.



By preserving the efficiency of porous-electrode models while injecting microstructure information, the workflow runs in minutes per design, enabling rapid screening and sensitivity analyses under fast (dis)charge. Combined with generative AI methods, it supports high-throughput exploration of electrode microstructure space for both Li- and Na-ion chemistries, accelerating discovery of architectures that improve transport, reaction uniformity, and capacity utilization.

Keywords: ModVal2026, tortuosity, microstructure-aware cell model, DFN model, battery cell simulation

Towards a predictive scale-resolved 3D model of sulfurized polyacrylonitrile (SPAN) batteries for aviation

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Abstract

Sulfurized polyacrylonitrile (SPAN) batteries are a recent promising representative from the class of Lithium-Sulfur batteries (LSB). The latter are often associated with aerospace electrification. However, traditional LSBs fail to fulfill the vital technical requirements of aviation at the same time, namely safety, reliability, energy and power. This is provably different for SPAN batteries as we could show in the BMFTR funded project SulForFlight (FKZ 03XP0491). Despite rather first obvious optimization steps, the developed pouch cells reached a maturity comparable to Lithium-Ion cells used in More Electric Aircraft (MEA) architectures. To tap the full potential in the near future and optimally balance the aforementioned requirements relevant for the harsh operating conditions faced in aviation, the development of a predictive scale-resolved 3D SPAN battery model seems natural. Our work focuses on carefully rationalizing the model development, why the 3D electrode structure matters and how it beneficially influences the SPAN cell characteristics.

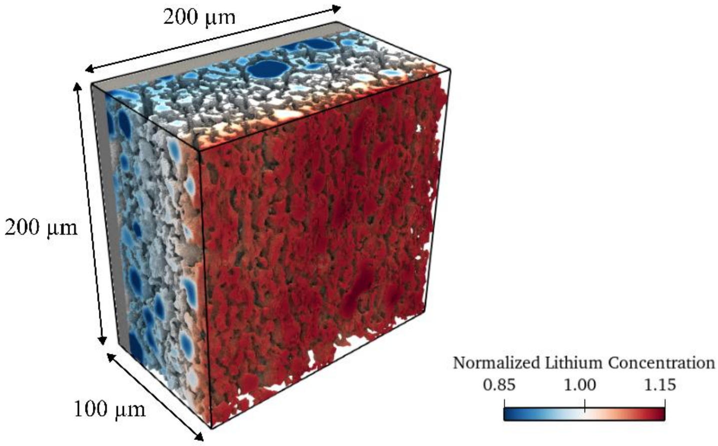

Figure 1: Normalized Lithium concentration at DoD=100% for 1C. The model comprises ~120 Mio. degrees of freedom (DOF) and the full discharge was computed on 1536 cores in 1.5h.

Keywords: SPAN Batteries, Lithium-Sulfur, Aerospace Electrification, High Performance Computing, Scale-Resolved Simulation

Nonlinear Battery Model in Frequency-Domain and its Parameterization

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Abstract

Thorough analysis of reaction kinetics in electrochemical systems, such as Li-Ion batteries, is a challenging task, mostly due to convoluted transport processes or side reactions.
The frequency dependence of the underlying processes can be used in Nonlinear Frequency Response Analysis (NFRA) to obtain excellent separability between different charge transfer processes and transport. In contrast to Electrochemical Impedance Spectroscopy (EIS) the nonlinear information is maintained, emerging as harmonic content in the voltage response, allowing unprecedented insights into charge transfer reactions (J. Ulrich et al., J Power Sources 647 (2025) 237358.).
Here, we present a fast-computing Doyle-Fuller-Newman-based model for Li-Ion batteries in frequency-domain (ωP2D), where nonlinearity and thus higher harmonics are included without any loss of model detail. The resulting system is a differential-algebraic system of equations, which is solved along the thickness of the battery electrodes using collocation. This approach enables a thorough parameterization of charge transfer kinetics using SOC-dependent NFR data of NMC811 and 622 half-cells. While the exchange current density resembles the dependence known from literature, NFRA additionally shows that intercalation becomes more and more asymmetric, the more the electrode is lithiated. Furthermore, based on the third harmonic response, we detect that, contrary to Butler-Volmer kinetics, charge transfer coefficients do not sum up to unity, highlighting the necessity for advanced kinetic models.

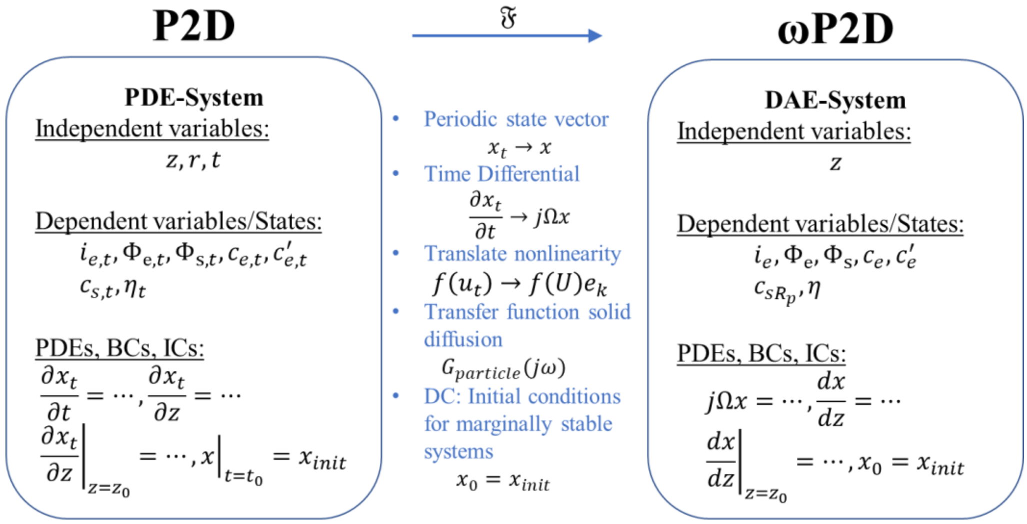

Figure 1: Scheme for translating the Doyle-Fuller-Newman model into the frequency-domain “ωP2D” model for periodic steady state

Keywords: ModVal2026, Impedance Spectroscopy, Nonlinear Frequency Response Analysis, Doyle-Fuller-Newman Model, Intercalation kinetics

Quantification of lithiation heterogeneities in graphite electrode under normal and fast charging conditions using phase-field modelling

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Abstract

Lithium intercalation in electroactive materials plays a key role in the electrochemical performance of batteries especially at fast charging rate. It determines the local state of charge of the particles during charging and influences the electrode kinetics. In addition, the electrode microstructure including the morphology of the active materials strongly affect cell performance. A deeper understanding of the mechanisms governing lithium transport and intercalation within electrodes under both normal and fast-changing conditions is therefore needed.

The Doyle–Fuller–Newman (DFN) pseudo-two-dimensional (P2D) model is widely used to investigate local phenomena such as electrolyte migration and diffusion, as well as charge-transfer reactions and ion intercalation in active materials. However, because of the complexity of electrochemical phenomena and the limitations of the model assumptions, modified P2D are needed.

To study the local behavior of a porous graphite electrode at two lenght scales—the particle scale and the electrode scale—we developed a model based on a modified P2D framework coupled with a phase-field approach and a volume-averaging method for porous media. This approach captures the phase transitions within graphite particles (figure 1.a) and provides a more accurate description of electrolyte field variables evolution (figure 1.b) under fast-changing conditions.

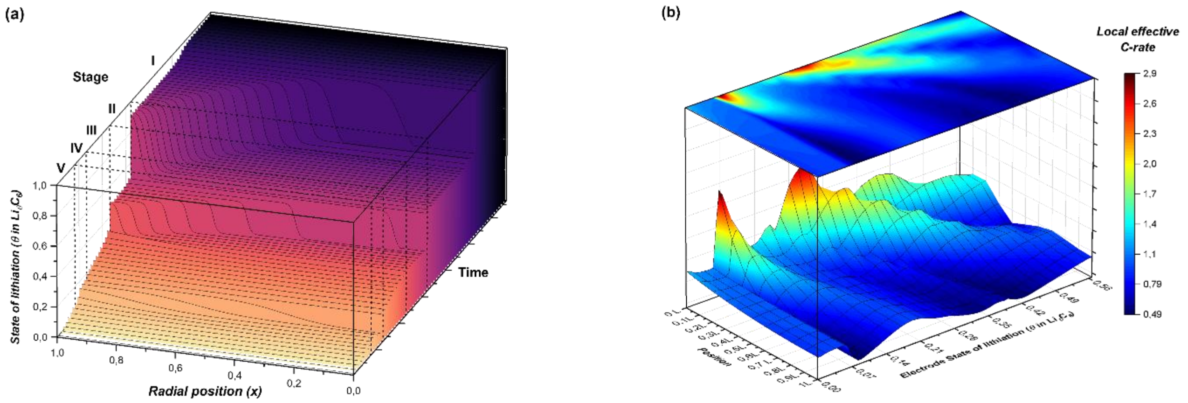

Figure 1. (a) Evolution of lithium stoichiometry inside graphite particle and (b) local effective charging rate during charge at 1C

Keywords: Batterie, Phase-field, Fast-charge, Modeling, Graphite

MODVAL 2026: 22nd Symposium on Modeling and Experimental. Validation of Electrochemical Energy Technologies
10 – 11 March 2026, Lausanne Switzerland

Low-complexity parameterization of a degradation-sensitive equivalent circuit model

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Abstract

The increasing deployment of lithium-ion battery systems in electric vehicles and stationary applications requires reliable methods to predict their lifespan. Equivalent circuit models (ECMs) offer an attractive balance between physical interpretability and computational efficiency. Conventional models, such as physicochemical models, machine learning models, and degradation mode models, often lack one of these attributes.

We present a degradation-sensitive, physics-informed ECM that integrates degradation modes (DMs), such as loss of lithium inventory (LLI) and loss of active material (LAM), with degradation kinetics[1]. The proposed model (Figure 1a) consists of: electrode specific open-circuit voltage sources, degradation-induced current leakage paths representing DMs, electrode-specific R–RC elements capturing dynamic and static resistive behaviour, and a series resistance accounting for electrolyte and current collector contributions. This ECM enables accurate lifetime prediction with minimal experimental input.

The model was parameterized for a 150 Ah prismatic LFP/graphite cell cycled at 1C and 35°C under CCCV conditions within the operational voltage window (Figure 1b). Degradation rate parameters were manually tuned to reproduce experimentally-identified degradation modes (Figure 1d, e), quantified using established methodologies[2]. The proposed ECM accurately predicts the observed capacity fade (Figure 1c), with degradation dominated by solid electrolyte interphase, SEI-induced LLI. The negative electrode potential remained above the lithium plating threshold, indicating the absence of lithium plating.

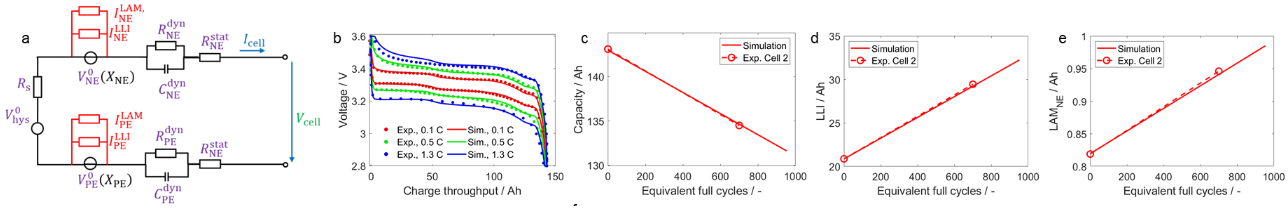

Figure 1: a) The ECM, b) begin of life model validation, c) capacity, d) LLI and e) LAM of NE as a function of the equivalent full cycles

1. Mmeka, P. O., Dubarry, M. Bessler, W. G. J. Electrochem. Soc. 172, 080538 (2025).
2. Mayur, M. et al. Phys. Chem. Chem. Phys. 21, 23672–23684 (2019).

Keywords: LLI, LAM, degradation modes, physics-informed ECM

Suppressing Phantom LAM/LLI in Voltage-Curve Degradation Mode Analysis via Ohmic IR Correction and Branch-Aware Hysteresis Handling

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Abstract

Degradation mode analysis (DMA) is widely used to attribute capacity fade to loss of lithium inventory (LLI) and loss of active material (LAM) from low-rate voltage–capacity data. However, the measured low-rate trace is a pseudo-OCV (pOCV) that retains two non-degradation contributions: (I) an SOC-dependent ohmic drop and (ii) intrinsic charge–discharge hysteresis, which is pronounced in graphite–silicon oxide (Gr/SiOx) negative electrodes. We show that these effects can dominate DMA attribution, producing “phantom” LAM/LLI—apparent material loss created by curve registration, branch choice, and voltage-windowing rather than true degradation. Using two commercial 21700 cells (LG M50T, higher resistance; Molicel P45B, lower resistance), we extract an SOC-dependent instantaneous resistance $R_{\Omega}(SoC)$ from the first ~50 ms pulse step and apply an ohmic-only IR correction prior to DMA fitting. In the LG M50T, IR correction lifts the discharge pOCV by ~+13–27 mV with ageing; omitting IR correction systematically under-diagnoses PE-LAM (down to −8.80% relative error at late life) and suppresses LLI (median −3.07%), with compensating inflation of apparent graphite loss. In the low-resistance P45B, hysteresis and window selection drive large charge–discharge divergences on a branch-fair 3.0–4.2 V window: at end-of-life, charge reports higher PE-LAM (+3.42 pp) and higher LLI (+5.36 pp), while discharge recovers substantially larger Si-LAM (discharge–charge difference +14.38 pp). Truncating the lower cutoff (2.5–4.2 → 3.0–4.2 V) under-reports Si-LAM by 13.61 pp by removing the Si-sensitive low-voltage tail. We conclude with a practical DMA protocol for Gr/Si systems: correct only the instantaneous ohmic term, enforce a harmonized voltage window, and base quantitative attribution primarily on the discharge branch.

Keywords: ModVal2026, Degradation mode analysis (DMA), Ohmic resistance / IR correction, Voltage hysteresis, Graphite–silicon (Gr/SiOx) electrode, Voltage-window sensitivity / curve fitting

Modelling of OCV Hysteresis

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Abstract

Open circuit voltage (OCV) hysteresis refers to the path-dependent difference in equilibrium open circuit voltage between charge and discharge at identical states of charge (SOC). Anode materials such as graphite and silicon show a hysteresis of 30 mV and 200 mV respectively while cathode materials such as LFP shows up to 30 mV. Modelling this is crucial not only for accurate voltage prediction, but also for state estimation in EVs thereby affecting its range prediction and safety. OCV hysteresis can be modelled using operator-based approaches like with the Preisach model, or differential equation based empirical approaches like with the Plett model. For EVs, where the use of pseudo-2D (P2D) models are very prevalent, the Plett model is more compatible owing to the similar differential equation-based framework of P2D models. While the Plett model is fully empirical and requires extensive parameterisation, some physics-motivated inclusion was achieved in the modified Plett model where the shapes of hysteresis transitions are captured from the differential capacity of the system, thereby significantly reducing the extent of parameterization. However, the Plett model and all its derivatives are accurate only for hysteresis transitions of the first order and fail to account for complex behaviours observed during higher order reversals and nested current loops. Such scenarios are frequently encountered by EVs especially during multiple recuperations. The limitations of the model originate from the innate asymmetry and simplicity of the differential equations used. In this regard, our work proposes physically motivated hysteresis representations achieved by correcting the Plett model and by incorporating experimentally observed closed loop and nested loop voltage responses. While the proposed models capture first order transitions with comparable accuracy to the Plett model, they show significantly higher accuracies with higher order transitions and successive recuperation pulses.

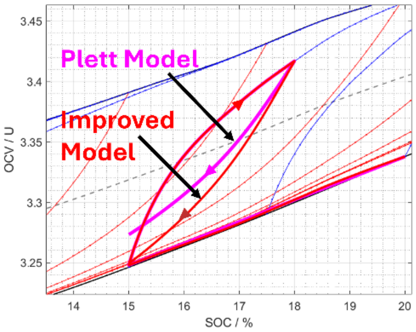

Figure 1: Simulation of a closed hysteresis loop where the Plett Model does not form a closed loop, contrary to experimental observations, and its correction in the improved model.

Keywords: ModVal2026, Hysteresis, Open Circuit Voltage, Plett Model

Oral Abstracts

Session B: Energy Conversion

Quantitative Analysis of Morphology and Performance of Electrode Microstructure in Solid Oxide Electrolysis Cells via Pore-scale Modeling

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Abstract

Solid-oxide electrolysis cells (SOECs) are a compelling route for high-temperature hydrogen production, and Ni-YSZ remains the conventional fuel-electrode material. Realizing the potential of Ni-YSZ electrodes requires simultaneous facilitation of gas diffusion, charge transport, and electrochemical activity, all of which are governed by electrode microstructure. Here, we reconstruct the three-dimensional morphologies of pristine and degraded Ni-YSZ fuel electrodes from FIB-SEM and develop a heterogeneous pore-scale multiphysics framework that resolves gas-phase species transport, electronic/ionic conduction pathways, and the spatial distribution of reaction rates in active triple-phase boundary (TPB) regions. The model quantifies how microstructural descriptors (phase connectivity, phase fraction, phase size, and TPB density), operating conditions (inlet gas composition and operating current density), and material properties (ionic conductivity) impact electrode performance. High local current density in active TPB regions concentrates near the electrolyte-fuel-electrode interface, and longer/more tortuous H_2O transport pathways reduce the local H_2O concentration at active TPB regions. Lower inlet H_2O decreases electrochemical activity at active TPB regions and further limits H_2O transport, increasing both activation and concentration (mass-transport) overpotentials. Increasing ionic conductivity expands the thickness of the electrochemically active reaction zone. After high-temperature operation for 10.7 kh, the degraded electrode exhibits reduced pore connectivity, pore volume fraction, and active TPB density, which amplifies the H_2O concentration gradient and increases the non-uniformity of local current density within the electrode. This framework provides quantitative insights into the coupled roles of microstructure, mass/charge transport, and kinetics, offering design rules for engineering durable, high-performance Ni-YSZ fuel electrodes for SOECs.

Keywords: Solid oxide electrolysis cell, Pore-scale modeling, Microstructure degradation

Multiphysics Simulation of Ni Agglomeration and Migration in Solid Oxide Cells under High-Steam Partial Pressure and Polarization Conditions

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Abstract

Commercialization of solid oxide cells (SOCs) for long-term operation requires mitigating Ni agglomeration and migration. Ostwald ripening and wettability changes are recognized as key mechanisms driving nickel agglomeration and migration [1]. Under high steam partial pressure and specific polarization conditions, variations in contact angle are governed by the local overpotential [2]. The overpotential is linked to the spatial distribution of Ni. Consequently, Ni evolution induces a dynamic redistribution of overpotential, which influences the degradation kinetics. However, although existing research methods can account for both microstructural evolution and mesoscopic electrochemical behavior, they are often weakly coupled, with feedback from the multiphysical fields not incorporated in real time into microstructure evolution modeling.

To bridge this gap, a framework which dynamically couples the phase field method (PFM) with computational fluid dynamics (CFD) is implemented in OpenFOAM® v2312 for microstructure simulation. In this coupled framework, PFM is used to simulate the evolution of Ni microstructure based on energy-minimization principles. CFD computes the spatially resolved multiphysics fields, including local overpotentials and steam partial pressure. The local Ni/YSZ contact angle variations are determined by spatial distributions of steam partial pressure and overpotential gradients [3]. These wettability changes are subsequently incorporated into the PFM to simulate the microstructural evolution of nickel. The resulting microstructural changes are then fed back into the CFD simulation via a level-set method.

In SOFC and SOEC modes, variations in current densities, steam partial pressure, and temperatures will lead to varying degrees of Ni agglomeration and migration. The coupled CFD-PFM approach enables predictions of the electrode's microstructural evolution and the resulting performance degradation after long-term operation. The results obtained by simulating these operating conditions can enhance the understanding of Ni agglomeration and migration and provide effective strategies to mitigate such degradation in SOCs.

Keywords: Multiphysics simulation, Ni agglomeration, Ni migration, wettability.

References:
[1] M. Trini et al. Journal of Power Sources. 450 (2020), 227599.
[2] S. Ihara et al. Journal of Power Sources. 654 (2025), 237867.
[3] Y. Shang et al. Journal of Power Sources. 661 (2026), 238577.

Development of 3D model for proton conducting ceramic electrolysis cell

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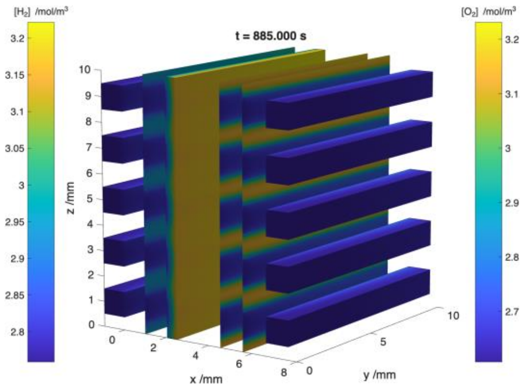
Abstract

Protonic Conducting Ceramic Electrolysis (PCCEL) is a promising technology for clean hydrogen production. Compared to high temperature Solid Oxide Electrolysis Cell (SOEC), the PPCEL is relevant for hydrogen production, processing and conversion at temperatures between 400°C and 600°C, which is typical for many industrial processes, e.g. refinery. From the modelling point of view, the PCCEL provides a challenge as multiple charge carriers can be active in the conducting ceramics, such as protons, oxygen vacancies and electrons. Furthermore, they feature complex incorporation kinetics and transport processes.

In this presentation our current state of the model development for PCCEL is reported. The transient model spatially resolves cell composite layers as well as the gas channels. Within each cell layer multiple physical phases are considered. The model features multi-step charge transfer and incorporation kinetics. For modelling of realistic operation conditions, a 3D model is indispensable due to gas concentration gradients along the channels and beneath the land. However, due to computational overheads, the direct usage of the 3D model is not feasible for a model parametrisation. It is more practical to use low dimensional models for this purpose but the applicability range must be investigated. We show how 1D and 2D models can be generically formulated for an increased applicability range.



Keywords: 3D model, proton conducting ceramic, electrolysis cell, dimensionally effects

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Spatially-resolved local electrochemical performance of solid oxide electrolysis cell: the effects of steam supply and polarization

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Abstract

Understanding the in-plane inhomogeneity of local electrochemical and multiphysical properties over a solid-oxide electrolysis cell is critical to reveal the bottleneck of enhancement of its real-world performance. However, due to high-temperature and sealing-demanding operating conditions, the experimental investigation usually performed on electrode-segmented cells is still largely limited and scarce, particularly on the perspective of electrolysis mode. This study first formed standardized protocols of electrochemical characterization of segmented solid-oxide cell to ensure the reliability of testing compared to non-segmented cells, and then investigated, based on a anode-segmented cathode-supported cell, the effects of steam supply and operating voltages on the in-plane distribution of multiple measurable properties, i.e., temperature and current density, as well as the driving elementary electrochemical processes.

The results show that the current density decreases along the steam flow direction with a maximal deviation of 61% under 4 sccm/cm^2 steam, which reduces to 45% when increasing steam flow to 10 sccm/cm^2, indicating sufficient steam supply promotes inhomogeneity of current density. Below 1.3 V, the local resistance increasingly along the steam-flow direction with a maximum resistance between segments not exceeding 4%. When the operating voltage reaches 1.5 V, intensified steam consumption in the inlet segments induces steep reactant gradients and increased flow field inhomogeneity, resulting in the maximum polarization resistance occurring at the middle segments. A higher operating voltage amplifies spatial inhomogeneous distribution of current density and electrochemical performance properties.

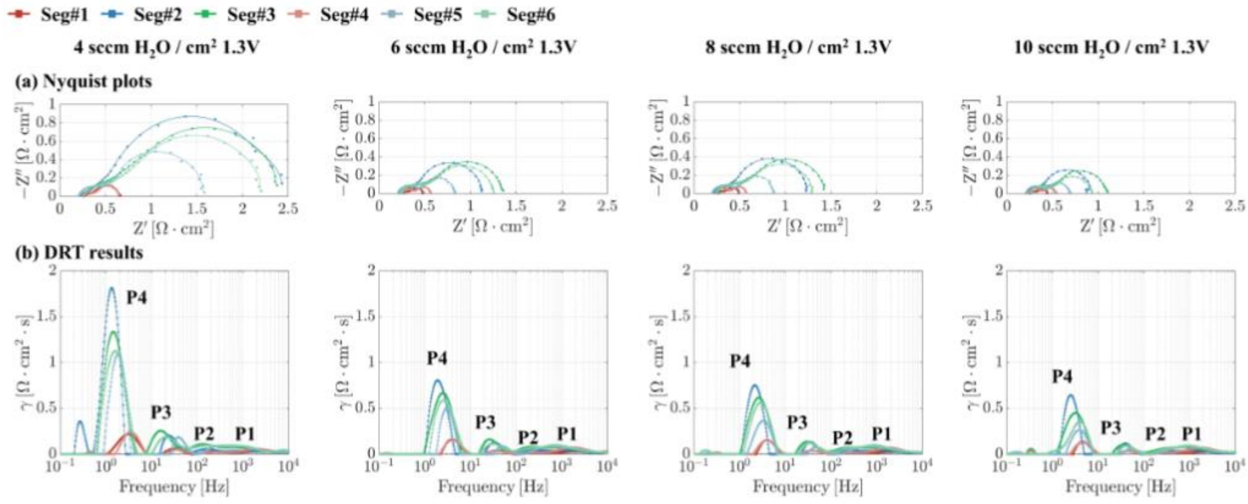

Figure 1. Impact of steam flow rates on local electrochemical performance: (a) Nyquist plots, and (b) DRT results

Impedance-based Performance Analysis and Modeling of Pressurized SOFCs for Aviation

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Abstract

The operation of SOFCs in pressurized conditions improves performance and enables coupling to a gas turbine, making this hybrid concept particularly relevant for aviation applications. To support system design and guide stack and cell optimization, existing physicochemical SOFC performance models [1] must be adapted for pressurized conditions and validated accordingly.

In this contribution, a high-performance planar anode-supported incremental cell (1 cm^2) was characterized in a recently developed pressurized test bench [2] by impedance spectroscopy and IV-characteristics up to 11 bar$_a$. By means of DRT analysis and subsequent CNLS-fitting to a physicochemical meaningful equivalent circuit model, the impact of pressure on the different loss mechanisms in the cell was evaluated and quantified. Based on this, an established 0D dc performance model [1] was parameterized and validated by IV-characteristics. The integration of this 0D approach into a 1D model [3] further enables to evaluate the performance on a stack cell level along the gas channel, considering gas conversion and temperature gradients.

We will show the impact of pressurization on impedance spectra, DRT and the obtained equivalent circuit model parameters, discuss necessary model adaptions and show the models validity for pressurized conditions. With the application of this validated 0D approach in a 1D along the channel model, the impact of pressurization on stack level was evaluated and suitable operating regimes were determined for a hydrogen powered SOFC in an integrated power and propulsion system for airborne applications.

References

[1] A. Leonide et al., *ECS Trans.*, **19**(20), (2009) 81.
[2] C. Grosselindemann et al., *J. Power Sources*, **614**, (2024) 234963.
[3] D. Klotz et al., *J. Power Sources*, **259**, (2014) 65 – 75.

Keywords: solid oxide fuel cell, aviation, pressurized operation, impedance analysis, 1D performance model

Design guidelines for ceria-based fuel electrodes: Connecting 3D microstructure and cell performance

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Abstract

Gadolinia doped ceria (GDC) combines high ionic conductivity in oxidizing atmospheres and mixed ionic electronic conductivity under reducing conditions as well as catalytic activity for hydrogen electrooxidation [1]. These intrinsic features make it an essential material for various components in state-of-the-art solid oxide cells [2]. Applied as a fuel electrode, GDC is typically mixed with nickel, analogous to the conventional Ni/yttria stabilized zirconia (YSZ) electrode. Compared to YSZ, GDC is able to extend the electrochemically active zone from the triple phase boundary to the entire GDC surface and can provide local electronic conductivity, which reduces the importance of a well percolated nickel matrix [3,4]. However, the relationship between microstructure and performance remains insufficiently understood.

In this work, eight symmetrical GDC-based fuel electrode cells with distinct microstructures, including nickel decorated variants [4], were fabricated, characterized by electrochemical impedance spectroscopy (EIS) and examined using scanning electron microscopy and focused ion beam (FIB) tomography. One of the key tools, when it comes to impedance analysis is the application of a physicochemically motivated transmission line model [4,5], which is parametrized in this study by conductivity data from four-point dc measurements, microstructural data from FIB tomography and electrochemical parameters derived from EIS. After a successful validation against experimental results, the model is used (i) to analyze relations between microstructure and individual parameters contributing to the polarization resistance and (ii) to simulate impedance and distribution of relaxation times (DRT) spectra for optimized electrode designs varying in microstructure and thickness at designated operation conditions.

The presented model features a powerful tool for model-aided solid oxide cell development, providing a guideline for designing GDC-based fuel electrodes with tailored microstructures that enhance electrochemical performance.

[1] Mogensen et al., *Solid State Ionics* 129 (2000) 63.
[2] Lenser et al., *J. Power Sources* 541 (2022) 231505.
[3] Kullmann et al., *J. Electrochem. Soc.* 171 (2024) 044511.
[4] Kullmann et al., *J. Power Sources* 625 (2025) 235621.
[5] Kullmann et al., *J. Power Sources* 587 (2023) 233706.

Keywords: solid oxide fuel cell, transmission line model, Ni/GDC, focus ion beam tomography, distribution of relaxation times, 3D microstructural analysis

Modeling of liquid water transport in fuel cell gas channels based on contact angles

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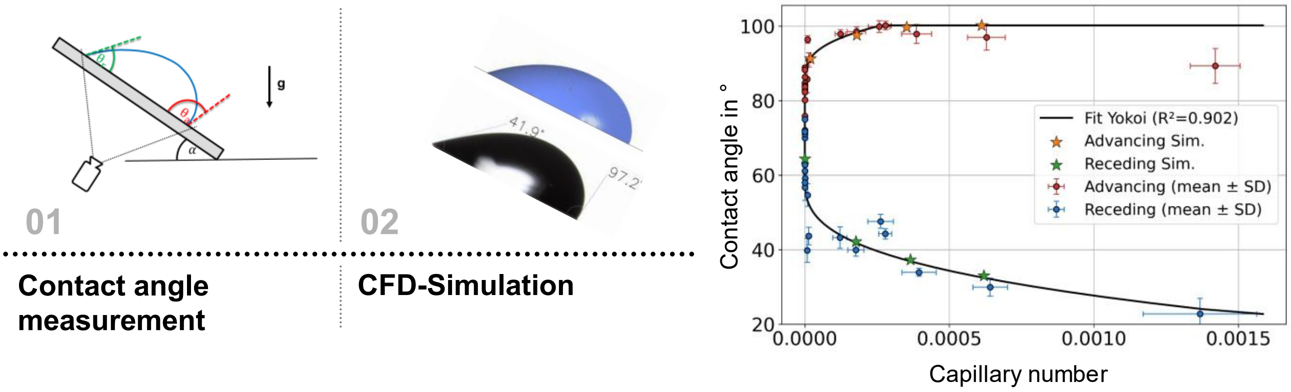
Abstract

The efficient operation of proton-exchange-membrane (PEM) fuel cells requires appropriate water management, which comprises two major aspects: (i) the maintenance of sufficient membrane humidification and (ii) the removal of liquid product water that accumulates in the gas channels. The most relevant two-phase flow regimes observed in the channels are droplet, slug, and film flow [1]. The transport of liquid water through the channels is strongly influenced by interactions with the channel walls. These interactions can be characterised through experimental means, for example by measuring the contact angles of a substrate-fluid pair at rest and in motion.

To determine suitable operating conditions for water removal in future aircraft fuel cell systems by CFD simulations, we evaluate whether incorporating dynamic contact angle correlations allows for an accurate description of liquid-water transport using the Volume-of-Fluid (VOF) method with the Ansys Fluent 2025R1 CFD solver. The measurement of contact angles, exemplified here for the polycarbonate-water pairing, is conducted optically on a dedicated test rig (Figure 1, left). Utilising this data, a correlation is derived between contact-line velocity and contact angle, employing the empirical model proposed by Yokoi [2]. The calibrated correlation is implemented in Fluent as a user-defined function (UDF) and initial CFD simulations are conducted for model validation (Figure 1, middle). The calibrated contact-angle model, the measured data points and the CFD results show good agreement (Figure 1, right), indicating consistency between experiment and simulation. Based on these findings, this approach will be extended to fuel cell relevant materials and applied to channel-scale simulations to study water removal, pressure loss and slip in the two-phase flow.



Contact angle measurement

CFD-Simulation

Figure 1: From left to right, the schematic test rig for the optical measurement of contact angles, an exemplary CFD-result, and the experimental and simulated results of the relationship between contact angle and capillary number are presented.

References:
[1] Lu, Z., et al. "Water management studies in PEM fuel cells, Part II: Ex situ investigation of flow maldistribution, pressure drop and two-phase flow pattern in gas channels." *Int. J. Hydrog. Energy* 34.8 (2009): 3445-3456.
[2] Yokoi, Kensuke, et al. "Numerical studies of the influence of the dynamic contact angle on a droplet impacting on a dry surface." *Physics of Fluids* 21.7 (2009).

Keywords: two-phase flow, liquid water transport, contact angle, VOF, PEM fuel cell

Numerical framework to study structural wetting properties of proton exchange membrane fuel cell catalyst layers with manufacturing parameters

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Abstract

Low temperature proton exchange membrane fuel cells are seen as a viable tool to decarbonate heavy duty vehicles for long-haul transport, but need improved performances and durability with lower cost for commercial attractiveness. A PEMFC is composed of various components, with extensive research made on the Cathode Catalyst Layer (CCL) as it holds central importance for performances. Under normal operating conditions, liquid water can form and accumulate in CCLs, hindering reactants transport and blocking reactive sites. Experimentally, visualizing liquid water transport in CCL is difficult. Modeling tools are necessary but current works still lack accurate pore-scale description for studying microstructure two-phase transport properties relations with manufacturing parameters.

Here, we developed a 3D microstructural resolved numerical framework to uncover two-phase dynamic relations with manufacturing parameters, as well as studying the influence of local wetting properties per solid phase. A previously developed discrete element method model is used to generate 3D CCL structures from four manufacturing parameters input and is coupled with state of art phase-field Lattice Boltzmann model for two-phase characterization [1]. Microstructural parameters such as relative permeability and water retention curves can be recovered.

As a proof of concept, the influence of solvent composition, more precisely fraction of water to isopropanol, was studied. Surface wettability influence was also studied by setting a proper contact angle for each solid phase. While showing clear trends, results can be implemented in upper scale model for direct quantitative performance estimation.

Keywords: Proton exchange membrane fuel cells, two-phase, cathode catalyst layer lattice Boltzmann method, discrete element method

Reference: [1] S. B. Vijayaraghavan, M. Baldofski, and A. A. Franco, Dec. 1, 2025, *J. Power Sources,* doi: 10.1016/j.jpowsour.2025.238238.

Optimization of a hybrid battery-supported fuel cell propulsion architecture for a 4 MW regional aircraft

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Abstract

The aviation sector faces critical sustainability challenges driven by ambitious European decarbonization targets, including up to a 75% reduction in CO_2 emissions per passenger by 2050. As conventional propulsion systems approach their efficiency limits, hybrid-electric architectures are emerging as viable alternatives. This study presents the preliminary sizing and optimization of a hybrid propulsion system combining proton exchange membrane fuel cell (PEMFC) and lithium-ion battery (LiB) applied to a regional aircraft. A representative mission profile was scaled to a 100 kW peak power level for preliminary sizing, enabling the definition of power requirements, degree of hybridization (DoH), and thermal loads across flight phases. Two hybridization strategies were analysed: direct hybridization without DC/DC conversion and indirect hybridization with a DC/DC converter. The direct configuration proved optimal, achieving a total propulsion system mass of 207 kg, compared to 277 kg and 327 kg for the indirect and non-optimized cases, respectively. This was enabled by a balanced power split, reducing thermal peaks and cooling system size. Advanced thermal management solutions, including phase change materials (PCMs) for battery cooling, led to significant reductions in thermal management system (TMS) weight and volume. Scaling the results to a 4 MW regional aircraft confirmed feasibility within existing maximum take-off weight (MTOW) limits, although with a reduced payload. Overall, the study demonstrates the potential of PEMFC–battery hybrid propulsion as a realistic pathway toward low-emission regional aviation.

Keywords: ModVal2026, electrification, aviation, hybrid propulsion, thermal management system.

Lattice Boltzmann model for volume-averaged fluid dynamics in heterogeneous non-Darcian porous media

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Abstract

We propose a lattice Boltzmann model (LBM) on standard lattices for simulating multi-dimensional, volume-averaged, weakly compressible, isothermal flow in isotropic, heterogeneous porous media, incorporating the Brinkman-Forchheimer extension of Darcy's law. Unlike prior LBM porous-media formulations, the model enforces the correct porosity scaling of both pressure and convective terms in the hydrodynamic limit, while preserving Galilean invariance and the isotropy of the viscous stress tensor. Linear and nonlinear drag, variable-porosity corrections, and additional body forces are incorporated through a consistent generalized forcing scheme. The model also allows independent specification of the temperature, and hence the speed of sound, improving computational efficiency, and includes a freely tunable bulk viscosity that can be used to enhance numerical stability. Model performance was evaluated via temporal spectral analysis and standard 2D benchmarks.

The ability to handle both channel regions and heterogeneous porous media enables a wide range of fuel-cell applications, including predicting in-plane and through-plane permeability over a range of flow rates, studying pressure-driven flow over permeable surfaces, and investigating flow bypass in serpentine and interdigitated channel designs. By providing a physics-resolving yet efficient alternative, the model is intended to accelerate early-stage design by replacing and/or complementing experimental studies. It also extends beyond simplified one-dimensional permeability-extraction models, which become unreliable at higher flow rates, where channel–porous media interactions can no longer be neglected and may lead to erroneous permeability estimates.

Keywords: ModVal2026, lattice Boltzmann method, heterogeneous porous media, volume-averaging, non-Darcian flow simulation, fuel cell materials design.

Pore-Scale Modeling of Through-Plane Reactive Transport in PEM Fuel Cell Electrodes with Optimized Mesoporous Carbon Supports

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Abstract

A pore-scale model based on the lattice Boltzmann method (LBM) is developed to simulate reactive transport processes across the through-plane direction of the cathode catalyst layer (CL) in a proton exchange membrane (PEM) fuel cell. The CL microstructures are generated using a process-based approach that accounts for realistic mesoporous carbon particle, platinum (Pt) catalysts, ionomer, and multi-scale pores, while considering realistic aggregation of mesoporous carbon particles to mimic experimental morphologies. Key characteristics, including pore size distribution, phase connectivity, and active catalyst surface area, are analysed with emphasis on mesoporous features. The effects of critical parameters, such as Pt/carbon (Pt/C) ratio, ionomer/carbon (I/C) ratio, mesoporous particle size, porosity, tortuosity, and Pt distribution, are investigated in terms of oxygen concentration profiles, effective reactive area, and overall reaction rates. Building on prior validation of mesoporous carbons for reducing local mass transport resistance, this study optimizes mesoporous designs to minimize through-plane transport losses. Results demonstrate that appropriately tailored mesoporous carbon microstructures with optimized porosity and tortuosity protect Pt particles from ionomer poisoning through internal placement while ensuring high oxygen accessibility. This enables elevated oxygen reduction reaction (ORR) rates and ultra-low through-plane mass transport resistance compared to solid carbon supports. These findings underscore the importance of realistic mesoporous reconstruction and aggregation in CL fabrication, proposing an ideal microstructure that substantially enhances PEM fuel cell performance through superior Pt protection, ORR activity, and transport efficiency. These findings underscore the critical role of integrating mesoporous carbon supports into PEMFC cathode CLs, offering a promising pathway to substantially mitigate performance limitations and long-term degradation issues by enhancing durability, efficiency, and catalyst utilization.

Keywords: Mesoporous carbon, Pore-scale Modeling, Microstructure, Catalyst design

Spatially Resolved Impedance Analysis and Modeling in PEMFCs

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Abstract

The complex performance characteristics of polymer electrolyte membrane fuel cells (PEMFCs) are highly sensitive to operating conditions. In large-scale PEMFCs, unavoidable spatial gradients along gas channels, such as variations in reactant availability, humidity, and pressure, alter local electrochemical processes and internal resistances, thereby determining local performance.

A comprehensive understanding of the spatial distribution of losses and their dependence on operating conditions is essential for developing targeted material and operational optimization strategies. Electrochemical characterization and model parameterization are challenging due to pronounced nonlinear couplings and frequent overlap of relaxation phenomena in integral measurements.

To address these challenges, an optimized segmented-cell design is employed to enable high-precision local current density measurements and spatially resolved electrochemical impedance spectroscopy (EIS) along the gas channel. Impedance spectra are analyzed using the distribution of relaxation times (DRT), which deconvolutes loss processes by their characteristic time constants [1,2]. Subsequently, the data are fitted with a physically motivated equivalent circuit model (ECM) to quantify loss process-related resistances as functions of operating conditions and channel position [3].

In this contribution, we present the segmented cell setup and the proposed physically meaningful ECM framework. Spatially resolved distributions of loss contributions, including ohmic resistance (R_0), charge-transfer resistance (R_{ct}), ionic transport resistance (R_{ion}), and mass-transport resistance (R_{mt}), are determined and discussed for systematic variations in current density, relative humidity, and pressure. The resulting resistance distribution offers impedance-based insights into the influence of operating conditions on local limitations along the channel.

References:
1. H. Schichlein et al., J. Appl. Electrochem. 32, pp. 875-882 (2002).
2. E. Ivers-Tiffée et al., J. Ceram. Soc. Japan 125, pp. 193-201 (2017).
3. M. Heinzmann et al., J. Power Sources 558, 232540 (2023).

Keywords: ModVal2026, Segmented PEMFC, Spatially Resolved EIS, DRT, ECM

Modelling hydrogen permeation during run-in phase of PEM water electrolysis

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Abstract

Hydrogen permeation and crossover are of great importance in PEM water electrolysis, as they reduce the overall efficiency of hydrogen production and can lead to safety issues. Lab short-stack tests are conducted with two different membrane types (two samples each) over approximately 1,000 hours each. The experiments with different membrane types show a slightly different dependency of the H_2 in O_2 values on the current density. In all experiments a run-in effect is observed, characterized by an increase in H_2 in O_2 over the first few hundred hours, followed by stabilization.
The experimental data is interpreted using a two-step model-based approach. First, a state-of-the-art diffusion model is used. This shows an approximate doubling of the membrane mass transfer coefficient and the cathode catalyst layer mass transfer coefficient (see Figure 1). Additionally, there is a significant difference in the absolute values of the cathode mass transfer coefficient between experiments with membrane type 1 and type 2. This is surprising, as the different membranes are coated with the same catalyst layers. To address this discrepancy, convective transport due to electro-osmotic drag (EOD) is integrated into the model in the second step. The significant difference in the EOD coefficient between the two membrane types can explain a large part of the observed difference. The relative change in the coefficients over time remains unchanged as shown in Figure 1.

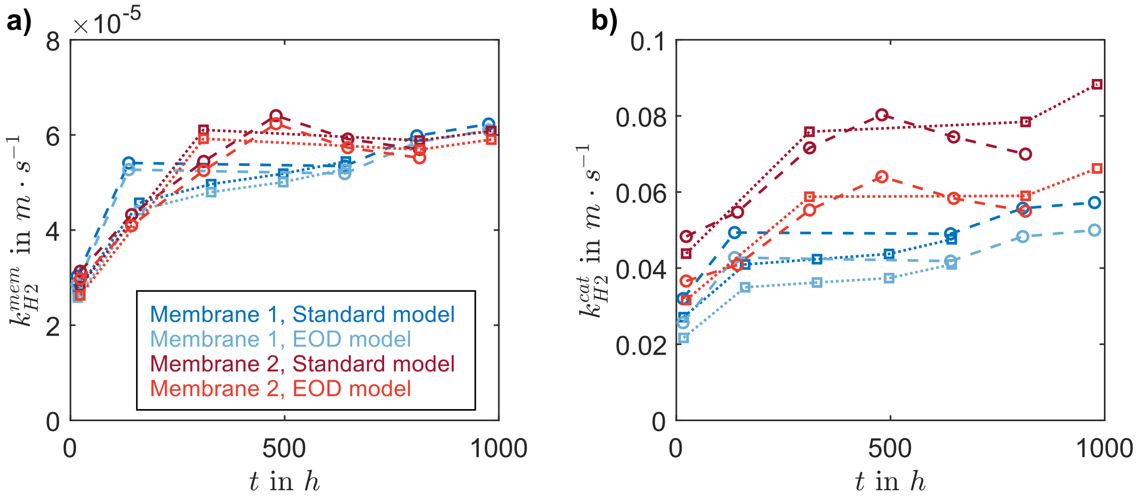

Figure 1: Fitted mass transfer coefficients using the standard model vs. using the EOD model depending on operating time (circles for Sample 1, squares for Sample 2): a) Membrane mass transfer coefficient, b) Cathode mass transfer coefficient

Keywords: ModVal2026, PEM electrolysis, Hydrogen crossover, Electro-osmotic drag

Multiphysics and Data-Driven Modeling of AC-Coupled PV–PEM Systems with Experimental Validation

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Abstract

Green hydrogen from renewable-powered electrolysis is a key pathway for decarbonizing the energy system, and proton exchange membrane (PEM) electrolyzers are particularly suitable for variable renewable energy (VRE) due to their fast dynamic response [1]. However, real PV–PEM deployments are rarely idealized: while DC coupling is often studied, the AC-bus coupling remains the dominant architecture in industrial and grid-connected systems, adding complexity through power electronics, controls, and balance-of-plant (BoP) subsystems [2]. In AC-coupled configurations, the AC–DC conversion can introduce ripple and harmonics that may affect stack durability, and intermittent solar operation drives rapid ramping, start–stop cycles, and extended partial-load operation where BoP parasitics can dominate efficiency [3]. Despite these realities, most published modeling studies rely on smoothed or idealized power profiles. Detailed multiphysics models can be accurate but computationally expensive, and machine learning (ML) approaches may lack validation on real AC-coupled systems and risk learning correlations rather than physical relationships [4].

To address this gap, this work investigates AC-coupled PV–PEM electrolysis under intermittent solar operation using rare, second-resolution experimental data provided by the Ranido facility in the Czech Republic, capturing realistic variability and fast transients. The experimental platform couples a PV system to a 0.34 Nm³/h PEM electrolyzer via an AC electrical bus, exposing the stack to inverter- and rectifier-conditioned power profiles while simultaneously accounting for BoP loads. A comprehensive dataset is collected, including meteorological conditions, PV/inverter outputs, electrolyzer operating variables, and hydrogen production, with operating regimes that include intermittency, ramping, and start-up/shutdown events.

Building on this experimental dataset, the present work focuses on the numerical analysis, modeling, and validation of AC-coupled PV–PEM operation through a three-layer modeling framework integrating measurement-driven characterization, high-fidelity physics-based and hybrid modeling, and fast data-driven emulation for scalable studies. First, a multiphysics PEM–BoP model is developed to reproduce behavior under intermittent AC-coupled inputs by coupling electrochemical losses with thermal dynamics, pressure effects, electrical losses, and auxiliary power consumption, explicitly emphasizing thermal inertia in transient voltage response. In parallel, a hybrid physics–machine-learning model is trained to reproduce PEM voltage dynamics under fluctuating current profiles using physically meaningful inputs while retaining interpretability, matching transient response. These two validated models capture system response with high fidelity, with a Normalized Root Mean Square Error (NRMSE) equal to 1.9% for the multiphysics model and a NRMSE that is equal to 1.6% for the physics-informed neural model.

Due to high-fidelity models can be computationally costly for long-horizon simulations, our work uses a neural-network emulator aimed at end-to-end prediction of hydrogen output from weather inputs alone. A PV emulator maps meteorological inputs to AC-side electrical power, and a PEM emulator maps available electrical power to hydrogen production, implicitly accounting for AC-coupling effects and BoP consumption, enabling scalable scenario analysis without continuous experimental operation. The key results demonstrate that both the multiphysics and physics-informed neutral networks (NN) models closely match experimental measurements, accurately reproducing voltage dynamics. The data-driven emulator predicts hydrogen production for representative days using only meteorological inputs, achieving R^2=0.84 and a relative total error below 4%. When tested on reordered weather sequences, the emulator preserves stable and physically consistent hydrogen production profiles, indicating robustness beyond simple time-series memorization.

In summary, this work delivers a validated, transferable pathway to analyze AC-coupled PV–PEM electrolysis under realistic intermittency by combining high resolution experiments with high-fidelity physics/hybrid models and a weather-driven emulator that enables efficient long-horizon system simulations.

Keywords: AC-coupled PV–PEM system; Green hydrogen production; Multiphysics modeling; Neural network emulation; Intermittent solar energy

References

[1] B. Yodwong, D. Guilbert, M. Phattanasak, W. Kaewmanee, M. Hinaje, and G. Vitale, “AC-DC converters for electrolyzer applications: State of the art and future challenges,” Jun. 01, 2020, *MDPI AG*. https://doi.org/10.3390/electronics9060912.

[2] E. Nguyen *et al.*, “Impact of short-term intermittent operation on experimental industrial PEM and alkaline electrolyzers,” *Int J Hydrogen Energy*, vol. 126, pp. 516–530, May 2025, https://doi.org/10.1016/j.ijhydene.2025.04.129.

[3] M. Mora, C. Bordons, E. López, M. A. Ridao, F. Isorna, and J. J. Caparrós, “Development and experimental validation of the dynamic model of an electrolyser for its integration with renewable generation,” in *2023 IEEE International Conference on Energy Technologies for Future Grids, ETFG 2023*, Institute of Electrical and Electronics Engineers Inc., 2023. https://doi.org/10.1109/ETFG55873.2023.10408325.

[4] A. Mohamed, H. Ibrahem, R. Yang, and K. Kim, “Optimization of Proton Exchange Membrane Electrolyzer Cell Design Using Machine Learning,” *Energies (Basel)*, vol. 15, no. 18, Sep. 2022, https://doi.org/10.3390/en15186657.

Development and Validation of a Layer-Unspecific Physical Model for Voltage Degradation and RUL Prediction in PEM Water Electrolyzers

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Abstract

Reliable lifetime prediction is becoming increasingly important as worldwide installed PEM water electrolysis (PEMWE) capacity is projected to reach 30 GWel by 2030. Existing degradation models, however, often lack applicability under real plant operating conditions, long-term validation, and quantified uncertainty, limiting their use in prognostics and health management. To address this gap, we present a layer-unspecific physical voltage-degradation model that enables in-operation monitoring and remaining useful life (RUL) prediction using only current–voltage data.

The method extracts quasi-steady polarization curves directly from operational data, eliminating the need for diagnostic downtime. As key novelty, a simplified electrochemical model with a fixed Tafel slope is fitted to each extracted polarization curve, allowing stable tracking of the temporal evolution of resistance and exchange current density while avoiding parameter collinearity. Their temporal evolution is described using constant, linear, or exponential regression, and parameter uncertainties are propagated via Monte Carlo sampling to obtain confidence-bounded voltage trajectories and RUL estimates.

The model is validated using (i) a 26200h synthetic dataset representing a 2.8MW PEMWE plant coupled to a wind turbine and (ii) a 2200h experimental six-cell PEMWE stack dataset. The synthetic dataset provides a known ground truth and tests the model's predictive capabilities under varied noise levels, whereas the experimental dataset confirms its applicability under real operating conditions. For both datasets, the model reproduces voltage values with millivolt-scale error and achieves prognostic horizons suitable for predictive maintenance. In both cases, it also differentiates degradation behavior and captures resistance-driven performance decline.

Overall, the results demonstrate a robust and plant-compatible approach for validating PEMWE degradation models, enabling long-term assessment, stable parameter extraction from operational data, and uncertainty-aware RUL prediction without the need for multi-year experiments.

Keywords: PEM water electrolysis, voltage decay, prognostics and health management (PHM), degradation model

Note: This work is currently under first revision as a full manuscript in the Journal of Power Sources.

Modeling of Anion Exchange Membrane Electrolysis: Investigation of the Dual Ion-Transport Pathways

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Abstract

Anion exchange membrane water electrolyzers (AEMWEs) are emerging as a promising technology for green hydrogen production. Unlike proton exchange membrane (PEM) systems, AEMWEs operate in an alkaline environment, enabling the use of cost-effective, non-noble catalysts and non-fluorinated anion exchange polymer membranes. However, due to less active catalyst, their performance is highly dependent on the concentration of the alkaline electrolyte and the use of thicker electrodes [1]. This results in more pronounced gas evolution challenges, including slow bubble detachment, bubble coverage, and gas accumulation—issues that are exacerbated at high current densities compared to PEM technology and can compromise the stability and durability of AEMWEs [2].

A key feature of alkaline membrane electrolysis lies in the dual ion-transport pathways, induced by the addition of an alkaline electrolyte [1]. Beyond reactions at the catalyst/ionomer interface, the liquid electrolyte enables reactions on catalytic surfaces not covered by the ionomer, thereby creating a second ion-transport pathway. This phenomenon introduces an additional ionic potential, promoting the transfer of charged species at the interface between the ionomer and the liquid electrolyte. Among the pioneering studies on this topic, Weber's research group developed a 1D multi-physical model incorporating this dual ion transport, relying on the Donnan equilibrium to describe the transfer of charged species at this interface [1].

In this study, we build upon this work by analyzing the impact of the dual ion-transport with 1D and 3D models. Our models explicitly solve charge balances and electrochemical reactions, providing a robust framework for analysis. We specifically investigate the influence of KOH concentration and ion-exchange kinetics on AEMWE performance. The results reveal significant performance variations depending on these parameters, which will be discussed through parametric studies.

Keywords: ModVal2026, Anion Exchange Membrane Electrolysis, Multiphysics Modeling, Dual Ion-Transport Pathways

[1] J. Liu, Z. Kang, D. Li, M. Pak, S.M. Alia, C. Fujimoto, G. Bender, Y.S. Kim, A.Z. Weber, *J. Electrochem. Soc.* **168** (2021) 054522.

[2] Shu Yuan, Congfan Zhao, Xiyang Cai, Lu An, Shuiyun Shen, Xiaohui Yan, Junliang Zhang, Bubble evolution and transport in PEM water electrolysis: Mechanism, impact, and management, Progress in Energy and Combustion Science, Volume 96, 2023, 101075, ISSN 0360-1285, https://doi.org/10.1016/j.pecs.2023.101075.

Multiphase Flow Experiments and Modeling of Shunt Currents in Alkaline Water Electrolysers

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Abstract

Shunt currents can significantly reduce the efficiency of bipolar stacks with liquid electrolytes, especially at low loads. To describe this, we developed an insightful approximate analytical model. In alkaline water electrolysers, gas bubbles strongly influence the outlet port- and return manifold resistances. To quantify this influence, we performed targeted experiments. Our results show that the gas fraction follows a drift-flux-like model, while its effect on resistance follows a Bruggeman-like relationship. Finally, Figure 1 shows how the shunt current measured in a short-stack increases with increasing liquid flow-rate. This is predicted well by our new multiphase shunt current model, providing a basis for optimizing future flexibly-operated electrolysers.

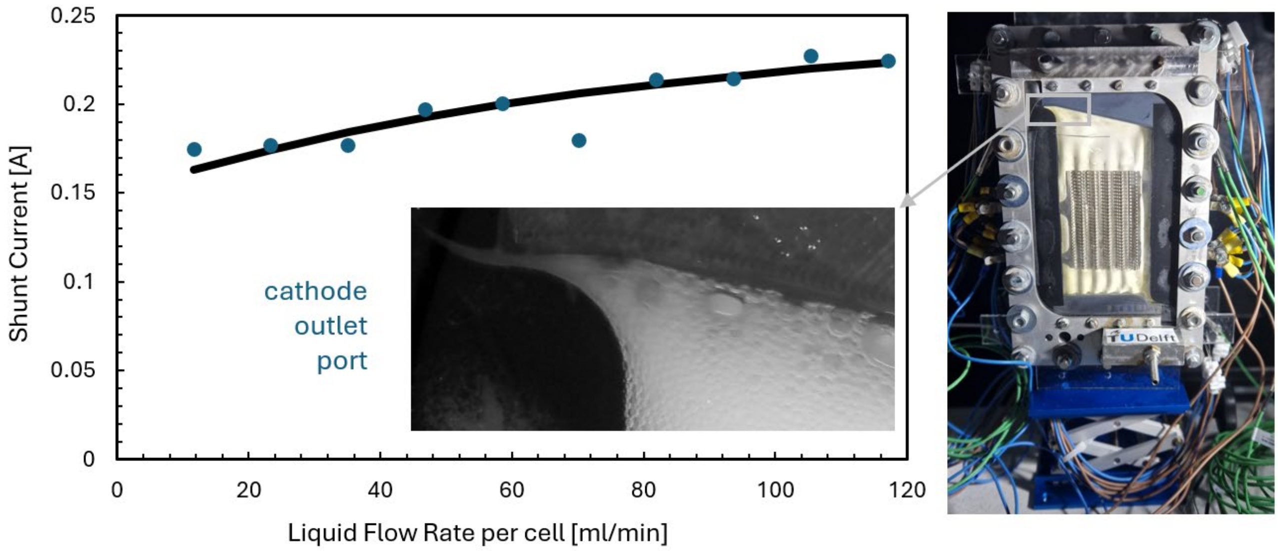

Figure 1: Measured (symbols) and modelled (solid lines) shunt currents - versus liquid flow rate in an in-house alkaline water electrolyser short-stack.

Keywords: Shunt Currents, Multiphase Flow, Alkaline Water Electrolysis, Analytical Model, Hydrogen Bubbles

A Novel CFD Model for AEM Electrolyzers

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Abstract

A comprehensive 3D CFD model for the performance simulation of anion exchange membrane (AEM) electrolyzers is implemented into a commercial CFD code [1]. The model features the following transport processes and reactions:

- Two-phase flow and gas species transport in channels and porous layers incl. phase change and capillary effects
- Heat transport in all regions and phases
- Dissolved water and gas species transport in membrane
- Ion and ionic charge transport in liquid phase and membrane
- Electronic charge transport in solid conductors
- Electrochemical reactions in catalyst layers (ionomer and liquid phase)
- Water and gas species transfer between fluids and ionomer in catalyst layer
- Ion transfer between liquid and ionomer in catalyst layer incl. **Donnan equilibrium**

Calculated polarization curves for different KOH concentrations are compared to measurements by Liu et al. [2] – see Figure 1 (left). The agreement between simulation and measurement is excellent in the whole current density and KOH concentration range. Figure 1 (right) shows the ionic current density in the membrane of an AEM cell with an interdigitated flow field geometry at a cell voltage of 1.9 V. The current density distribution results from the distributions of ion concentration, humidity and temperature.

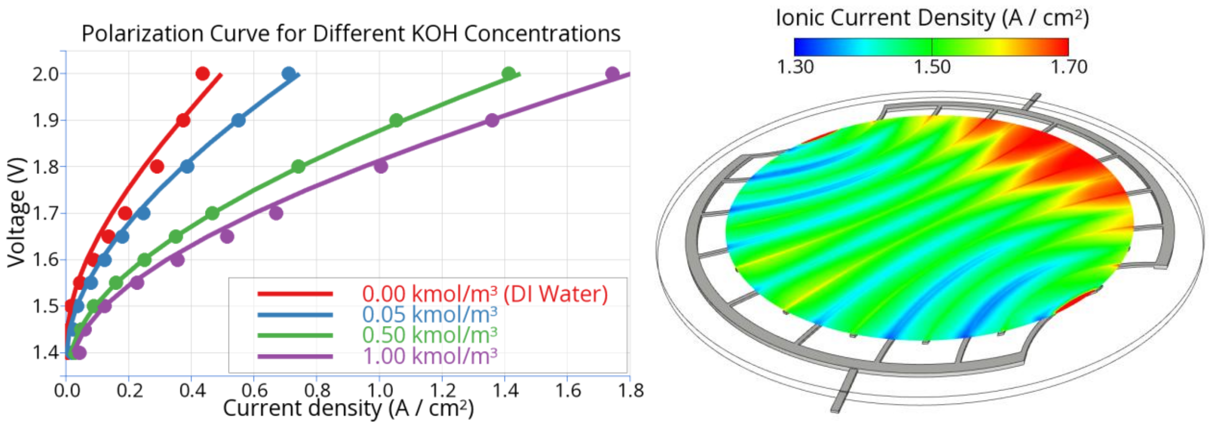

Figure 1: Left: calculated and measured [2] polarization curves for different KOH concentrations; right: ionic current density for interdigitated flow field geometry.

[1] AVL List GmbH, *FIRE M User Manual 2025 R2* (2025).
[2] J. Liu et al., *J. Electrochem. Soc.* 168, 054522, 2021.

Keywords: ModVal2026, AEM, AVL, FIRE M, CFD, Donnan

Transport properties of ammonia-saturated Nafion membranes

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Abstract

Proton transport in water is accelerated by the well-known Grotthuss mechanism, wherein hydrogen ions (i.e. protons) hop sequentially from water to water through the rearrangement of covalent and hydrogen bonds. As a result, the charge defect associated with an excess proton diffuses much more rapidly than ions that diffuse via vehicular transport. This phenomenon is essential to the efficient operation of traditional fuel cells, which utilize water as proton conducting layers within polymer membranes. Due to the limitations of aqueous fuel cells, there has been an effort to develop anhydrous proton exchange membranes (PEMs). Under certain conditions, ionic liquids, phosphoric acid, and ammonia can accept and donate a proton—like water—and can potentially participate in proton transport via the Grotthuss mechanism. Given the novelty of anhydrous PEMs, little is known about the transport properties and mechanisms in these materials. In this work, we use ab initio molecular dynamics (AIMD) to study ammonia and ammonium transport in ammonia-saturated Nafion and compare the results to experimental conductivity and diffusion measurements. AIMD is an electronic structure method which can explicitly handle bond breaking and formation, and can therefore accurately treat the physics of proton hopping. We will present simulation results on the formation of ammonia networks within the polymeric systems as a function of λ (where λ is the ratio of ammonia to sulfonate groups on Nafion), and the effects on ammonia and ammonium diffusion. As in aqueous systems, we find occurrences of Grotthuss hopping between ammonium and ammonia, occurring more frequently at lower λ values. In contrast to hydronium in water, however, we find that the diffusion mechanism of protons in ammonia is dominated by vehicular diffusion rather than structural diffusion via the Grotthuss mechanism. In this presentation, we will further elucidate the transport mechanisms of ammonium and ammonia, discuss the effect of phase separation between the polymer and ammonia, and outline several applications of ammonia-saturated polymer membranes.

Keywords: Charge transport modeling, ab initio molecular dynamics, AIMD, ammonia, polymer membranes

Pore-Scale Modeling of Electrochemical CO_2 Reduction within the Catalyst Layer of a Gas Diffusion Electrode

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Abstract

Designing and optimizing electrochemical systems, such as CO_2 electrolyzers, requires understanding of the local chemical environment and the coupled transport processes within the often complex porous architecture of the catalyst and its supporting layers.

The results presented are based on imaging data obtained via focused ion beam-scanning electron microscopy (FIB-SEM) tomography, thanks to which the porous structure of mesoporous materials can be reconstructed with resolution down to 4 nm. Typically, the sample preparation procedure, consisting in embedding of the material in epoxy, prevents to resolve C-based materials. An updated method including Cu-based metal complexes in the epoxy enables simultaneous imaging of an Ag-based catalyst layer (CL) and underlying microporous layer (MPL), allowing for the 2D segmentation and characterization of the CL/MPL interface. A coupled multi-physics pore-scale model, using the segmented cross-sections as domains, evaluates the effect of wetting regimes (ideally wetted, flooded pore-scale, flooded MPL, and flooded CFL) on overall GDE performances. A nonlinear dependence between wetting and performance is observed: current density and Faradaic efficiency drop sharply (one order of magnitude decrease in CO current density) when only the first few µm of MPL are flooded, decrease further (close to another order of magnitude decrease in CO current density) when the entire MPL (~90 µm) is flooded, and remain unchanged when flooding extends into the CFL. In the flooded pore-scale case, comparing two cross-sections reveals slight differences in CO current density, which we directly link to local morphological variations between site 1 and site 2. Local conditions at the OHP, including local CO_2 concentration and CO_2R current density, pH and 14-pOH, as well as their overall variability are examined. All the results are consistent with published experimental observations.

A detailed and locally resolved insight into the MPL–CL interface in a GDE for eCO_2R was obtained with a coupled experimental-numerical technique. The results provide a full quantification of local chemical conditions at the mesoscale, specifically at the OHP, within the CL of a real GDE, which are directly linked to the flooding state at the device level. FIB-SEM tomography, combined with simulations, enables detailed pore-scale resolution of operando conditions and 3D morphological characterization of CLs, improving the accuracy of device-scale GDE models.

Keywords: Electrochemical CO_2 Reduction, Gas Diffusion Electrodes, Pore-Scale Modeling, FIB-SEM Tomography, Wetting Regimes.

Effective Reaction Rates of Oxygen Reduction Reaction in Gas Diffusion Electrodes by First Principles Microscale Modelling

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Abstract

Gas diffusion electrodes (GDEs) are porous structures in which a liquid electrolyte is brought into contact with a gas phase in the presence of a conducting electrocatalyst. To prevent electrolyte breakthrough, hydrophobic components such as PTFE are finely distributed within the pore structure. The electrochemical reaction takes place close to the free surface between electrolyte, gas and electrocatalyst.

Current modelling of reaction rates rely heavily on fitted parameters and therefore lack predictive capability with respect to pore morphology or PTFE distribution. In this work, we present a rigorous, first principles-based route to overcome these limitations.

Using a digital twin of the GDE, we calculate the electrolyte distribution by pore network modelling and direct numerical simulations of pores with a stagnant free surface between electrolyte and gas. Using the fully resolved electrolyte distribution in pores with a stagnant free surface, we employ independently determined ORR kinetics from rotating-disc-electrode measurements reported by Kandaswamy et al. [1]. These three-dimensional simulations show that oxygen intrusion depth and reaction location depend sensitively on the applied overpotential. At technically relevant overpotentials, the ORR is confined to a narrow region around the gas–liquid–solid contact line, and local PTFE patches significantly influence this behaviour.

To enable efficient analysis across large pore ensembles, we derive a correlation that predicts oxygen consumption using an "equivalent elliptical pore", uniquely defined by the free-surface area and contact-line length of the real pore geometry. We show that although the local oxygen flux peaks near the contact line, the overall interface area contributes non-negligibly to the total flux. The flux exhibits no limiting behaviour but follows a logarithmic dependence on the Damköhler number, which is confirmed analytically for cylindrical pores. The resulting flux correlation, which is equivalent to the integral reaction rate, depends solely on the Damköhler number and geometric properties of the gas–liquid interface. The correlation predicts fluxes in full 3D simulations of real pore geometries with an accuracy of approximately 7% for $Da > 1000$.

This provides a pathway towards predictive GDE design optimization that explicitly accounts for mixed pore-wall materials.

Keywords: Gas diffusion electrodes, Oxygen reduction reaction, Pore-scale simulation

[1] Kandaswamy, S., Sorrentino, A., Borate, S., Živković, L. A., Petkovska, M., & Vidaković-Koch, T. (2019). Oxygen reduction reaction on silver electrodes under strong alkaline conditions. *Electrochimica Acta*, *320*. https://doi.org/10.1016/j.electacta.2019.07.028

Poster Abstracts

Session A: Energy Storage

Session A1: Diagnostics

Electrochemical-Model-Based Voltage Sensor Fault Diagnosis and Fault-Tolerant SOC Estimation for LFP Batteries

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Accurate state-of-charge (SOC) estimation is a fundamental requirement for the safe and efficient operation of battery management systems (BMSs). For lithium iron phosphate (LFP) batteries, however, SOC estimation remains particularly challenging due to the inherently flat open-circuit voltage (OCV)–SOC characteristic, which severely degrades system observability and amplifies the impact of modeling errors and sensor imperfections [1]. In practical BMS applications, voltage sensor faults such as bias drift and measurement noise are unavoidable and, if not properly addressed, can result in substantial SOC estimation errors.

This work presents a Residual Bias Compensation Dual Extended Kalman Filter (RBC-DEKF) framework for fault-tolerant SOC estimation of LFP batteries based on an electrochemical model. Unlike conventional bias-compensated Kalman filtering approaches that treat sensor bias as an augmented state within a single estimator, the proposed method adopts a decoupled dual-filter architecture. One extended Kalman filter (EKF) estimates the electrochemical states of a control-oriented single particle model with thermal effects (CPG-SPMT) [2,3], while a second scalar EKF independently estimates a residual voltage bias term. The estimated bias is used to continuously correct the voltage observation equation in real time, without perturbing the internal electrochemical state dynamics or introducing strong covariance coupling between states and bias.

Experimental validation is conducted using an A123 LFP 18650 cell under dynamic current profiles and varying temperatures [4]. In addition to nominal operating conditions, the robustness of the proposed approach is further evaluated under artificially injected voltage sensor faults, including constant voltage biases of ±30 mV combined with additive white measurement noise. These conditions are designed to reflect realistic sensor degradation scenarios encountered in practical BMS applications. The results show that the RBC-DEKF maintains accurate SOC tracking and effectively suppresses mid-SOC drift, whereas a conventional EKF configured with identical model structure and tuning parameters exhibits noticeable estimation bias and error accumulation.

Overall, this study demonstrates that residual bias compensation provides an effective and physically consistent mechanism for enhancing SOC estimation robustness in the presence of voltage sensor faults. The proposed framework offers a promising solution for fault-tolerant state estimation in LFP-based battery systems and provides a flexible foundation for future extensions toward integrated fault diagnosis and tolerant control strategies.

Keywords: Electrochemical modeling; Voltage sensor faults; Fault-tolerant estimation; Lithium iron phosphate; Battery management systems

References

1. Plett, G. L. (2015). Battery management systems, Volume I: Battery modeling. Artech House.
2. Guo, F., & Couto, L. D. (2025). Cpg-spmt: Control-oriented parameter-grouped single particle model with thermal effects for lithium-ion batteries. *SSRN 5344067*.
3. Guo, F., & Couto, L. D. (2025). A control-oriented simplified Single Particle Model with grouped parameter and sensitivity analysis for lithium-ion batteries. *Journal of Power Sources*, *649*, 237309.
4. CALCE Battery Research Group, A123 LFP 18650 battery dataset, University of Maryland. Accessed: Jan. 27, 2026. [Online]. Available: https://calce.umd.edu/battery-data/#A123

The secret life of e-scooter batteries

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Abstract

Shared light mobility based on electrified two wheelers (ETWs) has recently become a billion € industry with ~260 million e-scooter rides taken in Europe 2024 alone. Actors such as Lime (US), Dott (DE), and Voi (SE) have operated e-scooter & e-bike fleets for >7 years, and with these businesses becoming profitable, ETW use is likely to further expand. Given this, it is relevant to consider ways of benchmarking ETW battery performance, just as for any other electric vehicles. The automotive industry and customers benefit from standardised usage profiles, such as the Worldwide Harmonized Light-Duty Vehicles Test Procedure (WLTP), but at present no such profiles exist for ETWs. Furthermore, little is known about ETW-specific battery ageing, partly due to lack of detailed understanding of operating conditions, including a representative discharge profile, which arguably can have a significant impact on lifetime [1].

Here we approach the challenge of identifying typical ETW battery usage and load cycles that are relevant for both lifetime testing and performance benchmarking by using high frequency voltage, current, and temperature data collected from 10 thousand commercial e-scooters both during rides (> 10 million) and standby (>3 months accumulated resting). This way we can identify fleetwide distributions in C-rates, temperatures, rest times, and state-of-charge windows traversed. We are, furthermore, able to generate average fleet hour-by-hour power patterns for 71 different European cities; unique fingerprints for ETW power demand which can be used for time-series-clustering using dynamic time warping, identifying power demand archetypes.

Combining all above, we can tentatively give recommendations for representative test conditions and power profiles, similar to WLTP *etc.*, enabling accurate lab-testing of ETW batteries and future vehicle improvements.

References

[1] Geslin, A., Xu, L., Ganapathi, D. *et al.* Dynamic cycling enhances battery lifetime. Nat Energy 10, 172–180 (2025). https://doi.org/10.1038/s41560-024-01675-8

Keywords: Micromobility, Load profiles, Battery benchmarking, Battery degradation

Early Detection of Lithium Plating in Fast Charging Protocols for NMC Cells

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Abstract

Nowadays, fast charging is a common feature implemented in many devices. These aggressive charging strategies can lead to strong degradation phenomena and notably lithium plating. Detecting and mitigating lithium plating during fast charging is therefore crucial to improving charge acceptance while ensuring long-term reliability. In this context, the BFH leads the project AccelerateD Aging ProTocol for battEry Systems (Adaptes), aiming at reducing the duration of degradation tests and bridging the discrepancies between laboratory degradation and real-world usage.

Eleven different fast-charging scenarios were designed to induce varying degrees of lithium plating on commercial LG Chem 21700 M50LT lithium-ion cells. Under the three main plating-prone conditions (low temperatures, high C-rates, and high state of charge SOC), the cells were cycled in a temperature-controlled chamber using a battery cycler and periodically characterized with electrochemical impedance spectroscopy (EIS), incremental capacity analysis (ICA), and differential voltage analysis (DVA). Through OCV fitting and analysis of DVA and ICA, the computation of the degradation modes was realized. The distribution of relaxation times (DRT) was explored to identify lithium-plating-related signatures notably affecting the solid electrolyte interphase (SEI). Different post-mortem analysis strategies were conducted to validate the presence of lithium plating. Optical microscopy observations and scanning electron microscopy (SEM) imaging and Energy Dispersive Spectroscopy (EDS) mapping were initially utilized and could reveal only strong occurrences of plating. To overcome this flaw and comparatively quantify plating, a second approach with a portable glovebox in combination with XPS measurement techniques was performed to confirm the presence of lithium plating at the anode surface.

Finally, a pseudo 2D DFN physics-based model incorporating lithium plating mechanisms was adjusted to the experimental data using two different fitting approaches, first with time-series data and then with EIS. The objective of the model was to precisely indicate plating occurrences during fast charging. The EIS fitting strategy showed good agreement with the experimental results however, at medium C-rates, even under stripping current, the model lacked the characteristic impedance drop indicative of plating occurrences. Further investigation should be carried out to identify the parameters obscuring the typical impedance drop.

Keywords: Lithium plating, NMC, anode, accelerated ageing, post-mortem analysis

An original protocol to characterize electrode selective degradation mechanisms

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Abstract

Lithium-ion batteries play a crucial role in current decarbonization plans worldwide. To assess possible applications, whether first or second life, and to establish lifetime guarantees, a precise prediction of the battery's degradation is required. The difficulty for a proper assessment of aging has mainly lain in the complexity of the battery's internal environment and the significant number of possible degradation mechanisms and feedback interactions between the components and the byproducts of their degradation. Symmetrical cells have been used in the past to characterize the electrochemical behavior of active materials and electrolytes[1].; The present work proposes a similar aging study implementing negative-negative and positive-positive symmetrical cells as a means to partially contour these interactions and to isolate the phenomena taking place at each electrode. Symmetrical cells of LFP positive electrodes and graphite negative electrodes were studied in calendar ageing at different states of lithiation (therefore to different electrode potential values) and temperatures ranging from 35°C to 60°C. Results were compared with a set of regular pouch cells, studied under the same conditions of state of charge and temperature, allowing for validation of mechanisms observed in the symmetrical format, as well as showing the influence of cross-talk on degradation. This original approach to aging characterization should allow for better discrimination in degradation models proposed in the literature[2][3].

Keywords: ModVal2026, Lithium-ion, Battery, Aging, Degradation, Symmetric cell

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[1] Liu, Y.; Hamam, I.; Dahn, J. R. A Study of Vinylene Carbonate and Prop-1-Ene-1,3 Sultone Electrolyte Additives Using Polycrystalline Li[Ni0.6Mn0.2Co0.2]O2 in Positive/Positive Symmetric Cells. *J. Electrochem. Soc.* **2020**, *167* (11), 110527. https://doi.org/10.1149/1945-7111/aba36a.

[2] A Four Parameter Model for the Solid-Electrolyte Interphase to Predict Battery Aging during Operation. *Journal of Power Sources* **2022**, *539*, 231560. https://doi.org/10.1016/j.jpowsour.2022.231560.

[3] Physics-Based, Reduced Order Degradation Model of Lithium-Ion Batteries. *Journal of Power Sources* **2022**, *545*, 231900. https://doi.org/10.1016/j.jpowsour.2022.231900.

Understanding the Charge-Transfer Kinetics of LFP and LMFP Battery Cells

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Abstract

There is an ever-growing demand for more accurate health and performance estimation and modelling in battery applications such as electric vehicles. In recent years olivine cathode materials have had a renaissance owing to their stability, long lifetime, and operational safety [1]. Among these, lithium iron phosphate (LiFePO4) has been adopted in many electric vehicles (EVs) and stationary storage applications, with a theoretical capacity of ∼170 mAhg−1 [1]. Its low working potential (3.55 V vs. Li+/Li), however, is a limitation when applied in high energy density batteries [2]. The partial substitution of Fe with Mn increases the operating voltage as the Mn2+/Mn3+ redox reaction occurs at 4.1 V, providing a higher energy density than pure LFP [2,3]. To mitigate some of the challenges associated with pure LMFP cells, the cathode is often blended with other materials such as NMC, to give a “best of both worlds” approach. Key issues for pure LMFP include manganese dissolution, which shortens the lifetime of the battery; as well as reduced electrode kinetics at high Mn content due to the poor ionic and electronic conductivity associated with Jahn-Teller distortions [1,2].

In this project, the internal resistance of commercially available LFP and LMFP cells was investigated to characterise their dynamic electrical behaviour. Accurate knowledge of internal resistance is critical for assessing power capability and estimating state-of-health (SOH). The achievable energy and power density of batteries is limited by the internal resistance, which can be decomposed into: (i) ohmic resistance (R_0), associated with ionic and electronic conductivity as well as cell/electrode geometry, (ii) charge transfer resistance (R_{ct}), associated with reaction kinetics [4]. Two complementary techniques were used to measure the combined ohmic and charge transfer resistance of the battery cells; electrochemical impedance spectroscopy (EIS) and intermittent current interruption (ICI). EIS is a well-established tool for non-invasive electrochemical characterisation of cells and has the advantage of decoupling the different mechanisms in a cell based on their characteristic frequency. However, depending on the measured frequency range it can be a time-consuming measurement needing specialised equipment. ICI on the other hand, takes advantage of short rest periods (pulses) during a constant current (dis)charge to measure the voltage response during the pulses, offering a more time efficient alternative. In this study the temperature and rate dependence of the combined ohmic and charge transfer resistance (R_0+ R_{ct}) of LFP and LMFP cells were investigated via EIS and ICI, with both techniques yielding quantitatively comparable results. The evolution of resistance as a function of capacity throughput exhibited a unique profile that significantly differs from

that typically observed in NMC-based cells. While electrode reaction kinetics are conventionally described by the Butler–Volmer equation [5], this framework was extended to rationalise the atypical resistance behaviour observed in LFP and LMFP. Specifically, a modified two-site Butler–Volmer model was formulated in which two reaction sites (A and B) are simultaneously populated, each characterised by different reaction rates. Under applied current, charge transfer proceeds via preferential filling of either A or B sites, while the potential drop across the electrode–electrolyte interface remains uniform. The temporal evolution of site occupancy is governed by site-specific overpotentials that depend on the filling history of each site. The resulting two-site kinetic model was subsequently used to fit and interpret the experimental resistance data.

Keywords: ModVal2026, LFP, LMFP, charge-transfer kinetics

References:
[1] Gerard Bree et al. “Practical Pathways to Higher Energy Density LMFP Battery Cathodes”. In: Energy & Fuels (Feb. 2025). issn: 0887-0624. doi: 10.1021/acs.energyfuels.4c06201.
[2] Qiao Hu et al. “Revealing the voltage decay of LiMn0.7Fe0.3PO4 cathodes over cycling”. In: Nano Energy 123 (May 2024). issn: 22112855. doi: 10.1016/j.nanoen.2024.109422.
[3] A. K. Padhi, K. S. Nanjundaswamy, and J. B. Goodenough. “Phospho-olivines as Positive-Electrode Materials for Rechargeable Lithium Batteries”. In: Journal of The Electrochemical Society 144.4 (Apr. 1997), pp. 1188–1194. issn: 0013-4651. doi: 10.1149/1.1837571/XML.
[4] Rui Xiong, Linlin Li, and Jinpeng Tian. Towards a smarter battery management system: A critical review on battery state of health monitoring methods. Nov. 2018. doi: 10.1016/j.jpowsour.2018.10.019.
[5] Yu-Chuan Chien et al. “Rapid determination of solid-state diffusion coefficients in Li-based batteries via inter-mittent current interruption method”. In: (Apr. 2023). doi: 10.1038/s41467-023-37989-6.

AI for Batteries: Modelling, Testing and Operation

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Abstract

Battery aging, safety, and reliability remain critical barriers to the widespread deployment of next-generation energy storage technologies. Artificial intelligence (AI), when tightly integrated with physics-based understanding, offers powerful new opportunities to accelerate progress across the battery lifecycle. In this talk, I will present our recent work on developing digital twin technologies that span battery manufacturing, laboratory testing, and real-world operation.

Future battery diagnostics and prognostics increasingly depend on physics-informed machine learning (ML) to extract actionable insights from large-scale field data capturing coupled electrical, thermal, and mechanical behaviors. As embedded sensors for internal temperature and pressure monitoring become more affordable, they are being integrated into battery systems at scale, significantly expanding both the volume and diversity of available data. At the same time, these data streams are often noisy, incomplete, and sparsely sampled, posing substantial challenges for conventional modeling approaches. Data-driven and deep learning methods can reveal complex, nonlinear battery behaviors that are difficult to capture with first-principles models alone, while the incorporation of physical constraints improves interpretability, robustness, and generalization. Physics-based models remain essential in data-limited regimes and are increasingly adapted for field applications through AI-assisted parameter identification and calibration, particularly for large-format cells used in automotive and stationary energy storage.

This talk will outline a unified vision from industry and academia for integrating AI across modeling, testing, and operation of battery cells and systems. For modeling, I will focus on the development of data-driven and physics-informed models to capture complex battery behaviors beyond the reach of traditional formulations. For testing, I will present our work on machine learning-enabled, real-time optimization of experimental design. For operation, I will demonstrate how data-driven digital twins enable intelligent battery management using large-scale industry field datasets from automotive and stationary applications. Together, these advances point toward a new paradigm for AI-enabled, physics-informed battery engineering.

Keywords: Artificial Intelligence, Machine Learning, Battery, Physics, Data

Operando diagnostics of the open-circuit voltage curve of batteries with voltage-controlled models

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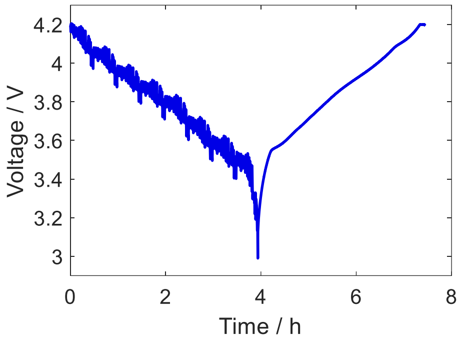
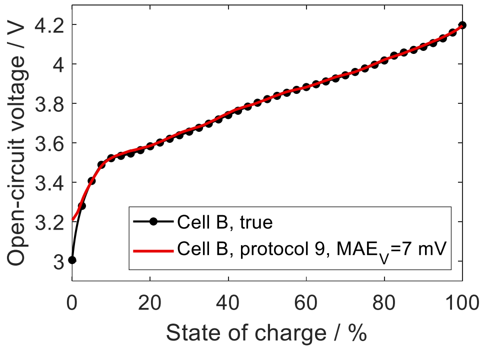
Abstract

The open-circuit voltage (OCV) curve is a key characteristic of lithium-ion batteries and essential for accurate state and health diagnostics [1]. Conventional OCV determination relies on low-current tests and long rest periods, which limits applicability under dynamic or operando conditions. Here we present a novel voltage-controlled model (VCM) approach for OCV estimation that operates directly on dynamic voltage and current data without requiring equilibrium conditions [2]. The method is based on an equivalent circuit model in which the measured voltage is used as input and the current is simulated as output. The deviation between simulated and measured current is iteratively used to estimate the OCV curve, starting from a simple linear initialization, until convergence. The approach was validated on four lithium-ion cells covering different chemistries (metal-oxide and iron-phosphate positive electrodes), formats, capacities (0.35–180 Ah), and aging states, using a wide range of experimental protocols including dynamic cycling (see upper figure), pulse tests, and long-duration multi-rate experiments. Across all datasets, the estimated OCV curves (see lower figure) showed high agreement with reference pseudo-OCV measurements, with mean absolute errors below 20 mV and an overall average of 10.1 mV. The proposed VCM-based OCV estimation eliminates the need for rest periods and low-current tests, enabling robust OCV identification under realistic operating conditions. Its applicability across diverse cell types and aging states makes it well suited for advanced battery modeling, real-time diagnostics, and integration into comprehensive battery management and validation frameworks.





[1] M. Dubarry and D. Beck, Energies 14, 2371 (2021), doi: 10.3390/en14092371.
[2] J. A. Braun and W. G. Bessler, “Diagnosis of the open-circuit voltage curve of batteries with voltage-controlled models,” Journal of Power Sources, submitted 2025.

Keywords: ModVal2026, Lithium-ion batteries, diagnosis, open-circuit voltage (OCV), voltage-controlled model (VCM)

Poster Abstracts

Session A: Energy Storage

Session A2: Manufacturing

An Automated Model Parametrization Framework for Microstructure Simulation of Electrochemical Devices

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Abstract

Electrochemical energy devices are vital for sustainable development, climate change mitigation, and ecological balance. They consist of electrodes and reaction species, where transport of these species is governed by various driving forces (electrochemical, diffusive, and mechanical) across multiple length scales. Particularly, the microstructure of electrodes greatly influences the accessibility of their active surface and their chemical environment throughout the device's operation. Since the microstructure is controlled by the manufacturing process, it is beneficial to simulate the process effects on microstructure to investigate their impact on its final properties. Various mesoscale simulation techniques, such as coarse-grained molecular dynamics (CGMD), the discrete element method (DEM), and the phase-field method, are employed to simulate the various process steps involved. However, the parameters of the models created with the simulation techniques require tuning and calibration, which can take considerable time if done manually. Hence, the automation of the model parametrization process for these simulations remains imperative.

In this work, a system-independent automation framework is presented, with optimizers such as the asynchronous particle swarm optimizer. It demonstrates the feasibility of high-throughput screening of model parameters for various processes used in different technologies, including fuel cells [1] and batteries [2], simulated using mesoscale DEM. The various optimizers used and methods for tuning their hyperparameters are detailed. Furthermore, each iteration of the optimizers, along with the final microstructure property achieved, is recorded. Complementary multivariate and machine learning analyses are then performed to identify the influencing parameters of the models for the various process simulations. This framework represents the next step in moving towards an ideal solution, enabling the determination of model parameters with only the target properties as inputs.

Reference:
1. S. B. Vijayaraghavan, M. Baldofski, A. A. Franco, *J. Power Sources* **2025**, *658*, 238238.
2. M. Alabdali, F. M. Zanotto, M. Duquesnoy, A.-K. Hatz, D. Ma, J. Auvergniot, V. Viallet, V. Seznec, A. A. Franco, *J. Power Sources* **2023**, *580*, 233427.

Keywords: ModVal2026, Electrode Manufacturing, Optimizer, Discrete Element Method

Poster Abstracts

Session A: Energy Storage

Session A3: Modelling

Insights into Battery Aging: Lessons Learned from Analyzing Public Datasets

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Conventional approaches for predicting the state-of-health (SOH) and remaining useful life (RUL) of lithium-ion batteries are primarily based on accelerated aging experiments combined with physics-based or data-driven models. Physics-based aging models explicitly describe degradation mechanisms such as SEI growth through governing equations, but they are computationally intensive and require detailed knowledge of electrochemical aging processes. In contrast, data-driven models offer faster computation and easier implementation, and recent advances in machine learning have demonstrated strong potential for SOH and RUL prediction by identifying complex patterns in high-dimensional battery data.

Recent data-driven studies increasingly rely on feature engineering, where raw cycling data are transformed into health indicators (HIs) prior to model training. Several studies have shown that carefully designed HIs—particularly those derived from voltage evolution in early cycles—can strongly correlate with battery lifetime. However, despite promising results, the generalizability of these HIs across different datasets remains largely unexamined. Differences in cell chemistry, format, capacity, and operating conditions may significantly influence HI performance, raising concerns about dataset-specific bias.

In this study, we systematically evaluate the robustness and transferability of extensively reported HIs across multiple large, open-source battery aging datasets. Building on the comprehensive dataset review by Mayemba et al.[1], six widely used datasets comprising diverse cell types and cycling protocols are analyzed. More than 40 HIs derived from voltage, current, temperature, time, and their first-order differentials are examined using various machine learning models. Our results show that voltage-based HIs—particularly those involving voltage differentials—consistently exhibit the highest predictive capability across nearly all datasets, while temperature-based features generally demonstrate limited effectiveness. Furthermore, our analysis reveals that categorizing HI performance based on cell properties and operating conditions is currently infeasible due to dataset scarcity, bias, and inconsistency, highlighting a critical limitation in existing open-source aging data and questioning common assumptions in smart battery management system design.

Keywords: Lithium-ion battery aging, Health indicators, Data-driven and machine learning models

1 Mayemba, Q., Mingant, R., Li, A., Ducret, G. & Venet, P. Aging datasets of commercial lithium-ion batteries: A review. *Journal of Energy Storage* **83**, 110560 (2024).

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Parameter Identification of Lithium-Ion Battery Equivalent Circuit Models Using GITT and EIS

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Lithium-ion (Li-ion) batteries represent a key technology in contemporary energy-storage systems due to their high energy density, long cycle life, and stable electrochemical performance [1]. Their application spans a wide range of sectors, including electric mobility, avionics, and stationary energy-storage systems, where reliable power delivery and accurate system-level modeling are of critical importance [2]. With the increasing deployment of Li-ion batteries in demanding operating environments, the development of accurate yet computationally efficient battery models has become essential for performance optimization, safety assurance, and lifetime prediction, as well as for advanced diagnostic and control functions within battery management systems [3].

Equivalent Circuit Models (ECMs) are widely employed to describe the electrical behavior of Li-ion cells, as they provide an effective representation of the underlying electrochemical processes with moderate computational complexity [4]. While lower-order ECMs are commonly used, their capability to capture complex dynamic behavior is limited when multiple time constants coexist within the cell [5, 6]. To address this limitation, a third-order ECM (3RC) is adopted in this work, consisting of an ohmic resistance and three parallel RC branches associated with fast interfacial phenomena, charge-transfer processes, and diffusion-related dynamics, respectively [7, 8].

The accuracy of an ECM strongly depends on the employed parameter identification method. This contribution investigates and compares two widely used approaches for ECM parameterization: the Galvanostatic Intermittent Titration Technique (GITT) and Electrochemical Impedance Spectroscopy (EIS). Both methods were applied to Li-ion cells under controlled laboratory conditions, and the parameters of the 3RC model were identified and analyzed. The comparison focuses on the fundamental differences between time-domain and frequency-domain parameterization, including experimental requirements, parameter interpretability, and resulting model characteristics.

The identified models were validated using real-world driving data acquired from the TU Brno Racing Formula Student electric vehicle. Both approaches achieved very good agreement between simulated and measured voltage responses (see Fig. 1), with root-mean-square errors of 9.86 mV for the EIS-based model and 9.61 mV for the GITT-based model. Although the difference in accuracy is marginal, the GITT-based model exhibited slightly improved performance under highly dynamic operating conditions. The results indicate that GITT enables reliable parameterization of higher-order ECMs without the need for specialized impedance measurement equipment, while achieving voltage response accuracy comparable to that obtained using EIS.

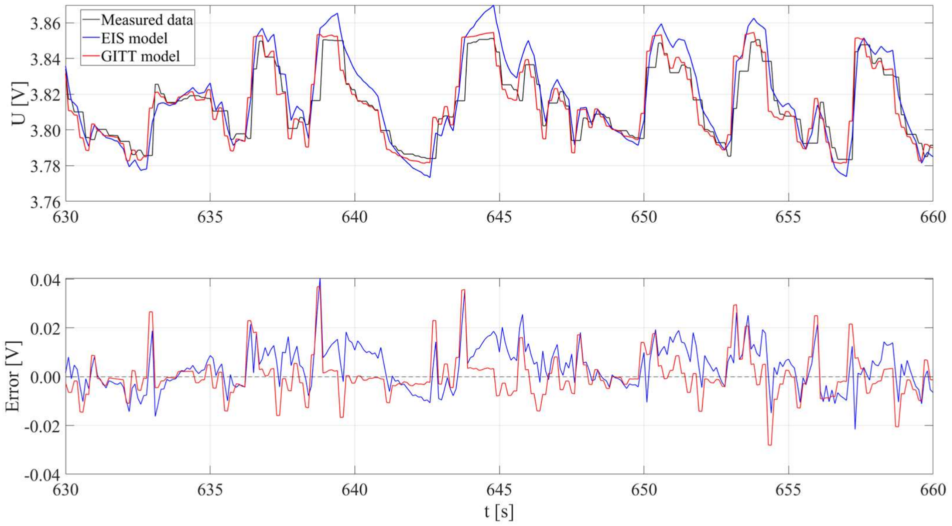

Fig. 1: Comparison of simulated voltage response using EIS and GITT

References:

1. A. A. Kebede, T. Kalogiannis, J. Van Mierlo, and M. Berecibar, “A comprehensive review of stationary energy storage devices for large scale renewable energy sources grid integration”, *Renewable and Sustainable Energy Reviews*, vol. 159, 2022, doi: 10.1016/j.rser.2022.112213.
2. M. M. Hasan *et al.*, “Advancing energy storage: The future trajectory of lithium-ion battery technologies”, *Journal of Energy Storage*, vol. 120, 2025, doi: 10.1016/j.est.2025.116511.
3. Y. Gao, M. Aziz, and S. Hussain, “Transfer learning-enhanced degradation modeling of lithium-ion batteries for predictive maintenance in stationary storage systems”, *Journal of Energy Storage*, vol. 141, 2026, doi: 10.1016/j.est.2025.118660.
4. A. Kulkarni, A. Nadeem, R. Di Fonso, Y. Zheng, and R. Teodorescu, “Novel low-complexity model development for Li-ion cells using online impedance measurement”, *Journal of Energy Storage*, vol. 91, 2024, doi: 10.1016/j.est.2023.110389.
5. F. Santoni *et al.*, “A guide to equivalent circuit fitting for impedance analysis and battery state estimation”, *Journal of Energy Storage*, vol. 82, 2024, doi: 10.1016/j.est.2023.110389.
6. N. Nicodemo, R. Di Rienzo, M. Lagnoni, A. Bertei, and F. Baronti, “Estimation of lithium-ion battery electrochemical properties from equivalent circuit model parameters using machine learning”, *Journal of Energy Storage*, vol. 99, 2024, doi: 10.1016/j.est.2024.113257.
7. J. Sun, Y. Liu, and J. Kainz, “A comparative study of parameter identification methods for equivalent circuit models for lithium-ion batteries and their application to state of health estimation”, *Journal of Energy Storage*, vol. 114, 2025, doi: 10.1016/j.est.2025.115707.
8. N. Meddings *et al.*, “Application of electrochemical impedance spectroscopy to commercial Li-ion cells: A review”, *Journal of Power Sources*, vol. 480, 2020, doi: 10.1016/j.jpowsour.2020.228742.
9. M. Sedlařík, P. Vyroubal, J. Lysák, M. Mačák, M. Šedina, and T. Kazda, “Comparison of Equivalent Circuit Model Parameterization Using GITT and EIS”, Nov. 2025, doi: 10.21203/rs.3.rs-7885669/v1.

Towards reproducible physics-based parametrization of lithium-ion batteries

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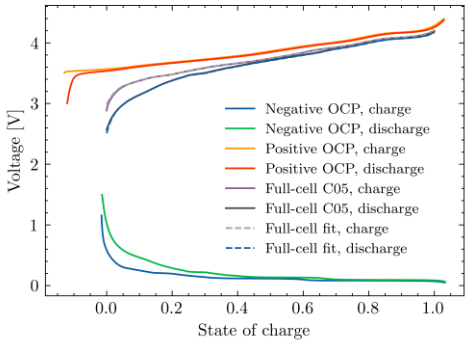
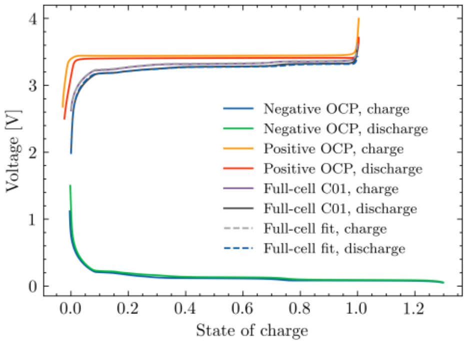
Abstract

Industry uses cell models for material selection and system design. For wide adoption, parametrization needs to be reliable, repeatable, and based on standardized procedures. Electrochemical models are more challenging to parameterize than equivalent circuits, having more states and coupled, nonlinear dynamics, but can reveal internal performance limitations (e.g. from transport) and make useful predictions via extrapolation. The impact of different processes on cell-level behavior must be isolated to ensure that parameter estimates correspond to intrinsic properties. Some processes are separated by timescale (e.g. using impedance) and others via their dependence on temperature, state-of-charge, and current.

In this poster, we present step-by-step optimization of the open-circuit, thermal, diffusion, and resistance parameters of two types of cylindrical lithium-ion battery cell (Gr-SiO_x/NCA, Gr/$LiFePO_4$). This extends our previous half-cell parametrization [1]. We employ a series of grouped-parameter models [2] to iteratively estimate identifiable parameters of the Doyle-Fuller-Newman model from, as far as possible, non-invasive measurements. We assess model and experimental limitations using PyBOP to optimize parameters in the time- and frequency-domains [3], including sensitivity analysis (Sobol indices, Hessian analysis), and deliver parameters in the Faraday Institution's Battery Parameter eXchange (BPX) format.





[1] R. Jackowska, N. E. Courtier, et al. J. Power Sources, 663:238881, 2026.
[2] N. Hallemans, N. E. Courtier, et al. J. Electrochem. Soc., 172:060507, 2025.
[3] B. Planden, N. E. Courtier, et al. J. Open Source Softw., 10(116):7874, 2025.

Keywords: Lithium-ion batteries, DFN model, parametrization, standardization.

Parametrisation of the equivalent hydraulic model

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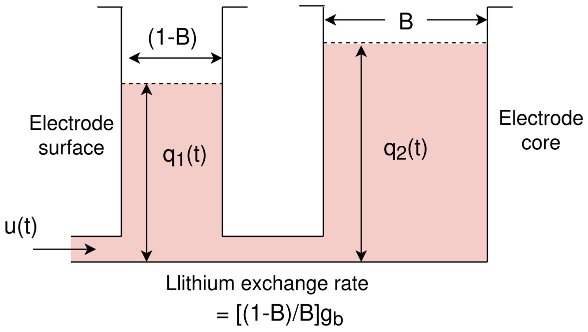
Abstract

Higher-order electrochemical models incorporate chemical, electrical, thermodynamic, and physical processes, in space and time, often resulting in non-linear, coupled differential-algebraic equations that are costly to solve and parametrise. On the other hand, reduced-order models such as the equivalent circuit model (ECM) can be easily parameterised and used in an online estimation and control framework. However, ECMs lack access to battery internal states and physical interpretability. Reduced-order electrochemical models, such as the single particle model, the single particle model with electrolyte, and the equivalent hydraulic model (EHM), are computationally efficient and can yield more transparent internal physical information. Also, because internal states are accessible, they can be coupled with degradation mechanisms to improve health prediction. In this work, we focus on parameterising the EHM as it offers an excellent trade-off between accuracy and complexity. The EHM assumes that the positive electrode dynamics are fast, and therefore can be ignored (only an overpotential associated with the positive electrode is required). It also assumes that the negative electrode dynamics can be described with a two-state model that includes the critical surface concentration (CSC) and (average) state of charge (SOC) as the states. A simple tank and pipe analogy can be made (see figure) relating states, although one might also think of them as basis functions describing the dynamics. The EHM complexity is similar to a two-state ECM, but the states couple into the output equation differently. The promise of the EHM is that it may be possible to find constant (not varying with SOC) parameters that describe behaviour over a wide range of conditions, unlike in ECMs, where often the parameters vary with SOC. In this work, we discuss parameterisation and validation of the EHM using the software PyBOP (Python Battery Optimisation and Parametrisation) against experimentally measured voltage responses with known open-circuit potential curves for each electrode.



Schematic of the equivalent hydraulic model

Keywords: Electrochemical models, Li-ion battery, EHM.

Modelling of battery half-cells consisting of $LiFePO_4$ considering mechanics and particle size distribution

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Abstract

$LiFePO_4$ (LFP) is one of the most commonly used battery materials due to its high safety, environmental sustainability, as well as relatively high theoretical capacity.

The goal of this work is to understand how the intrinsic properties of LFP influence the behaviour of a battery half-cell consisting of this active material. Modelling is a great tool to reach this goal, as it allows a detailed analysis of the processes going on in the battery during charging and discharging.

One established model for battery simulation is the Doyle-Fuller-Newman (DFN) model [1,2]. This model is able to capture the battery's behavior while still reducing the complexity to two one-dimensional levels - the electrode level, and the particle level. In this model, the active material particles are assumed to be spherical and to form a solid solution with the intercalating lithium ions, which can be modeled using Fickian diffusion.

While the DFN model works great for many active materials, it needs to be adapted to accurately capture the special characteristics of LFP.

When synthesized hydrothermally, LFP particles are platelet like, meaning they have large ac-facets and are comparably thin in the thickness (b-) direction. Therefore, in the work presented here, the particle shape of the model is adapted to these platelet-like structures. Another aspect considered is the anisotropic diffusion resulting from one-dimensional diffusion paths of the olivine crystal structure. These are oriented along the thickness direction of the particle, enabling the use of the depth-averaged approach to reduce the 3D-description of a LFP particle to 2D [3]. Furthermore, LFP undergoes phase-separation with a large miscibility gap leading to the long plateau in the charge and discharge curves of LFP. Therefore, the Fickian diffusion of the particle level of the DFN model is replaced by the Cahn-Hilliard-equation [4], which is suitable for modelling phase-separation in active materials.

The model has been further expanded to include anisotropic mechanics to simulate volumetric expansion as well as strains within the particles. Lastly, the model considers a particle-size distribution to show the possibility of particle-by-particle filling which has been reported widely for LFP.

[1] Newman, J. *Ind. Eng. Chem.* 1968, *60*, 12
[2] Newman, J.; Tiedemann, W. *AIChE J.* 1975, *21*, 25
[3] Bai, P.; Cogswell, D. A.; Bazant, M. Z. *Nano Lett.* 2011, *11*(11), 4890–4896
[4] Cahn, J. W. *Acta Metall.* 1961, *9*(9), 795–801

Keywords: DFN model, $LiFePO_4$, phase-field modelling

Thermodynamically consistent modelling of solid-electrolyte-interphase growth

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Abstract

Performance and lifetime of lithium-ion batteries are important parts of the decarbonization of transportation and energy grids. An accurate prediction of the degradation mechanism limiting them is crucial for optimizing their design and operating protocols. One major phenomenon is the growth of the solid-electrolyte-interphase (SEI), a passive layer that forms between the active material and the electrolyte [1].

We present a continuum model of SEI growth based on non-equilibrium thermodynamics, where the SEI is modelled as a mixed electron-ion conductor, and the interface between SEI and electrolyte as a moving boundary [2]. Transport laws and reaction kinetics are derived from electrochemical potential functions, ensuring thermodynamic consistency [3]. The result is a system of partial differential equations for active phase, SEI & electrolyte, and the interfaces between them. Under open-circuit conditions, we systematically derive a system of ordinary differential equations for the lithium concentration in the active material, the solvent concentration, and the SEI thickness.

Numerical simulations reproduce characteristic features that are observed experimentally, such as different growth regimes, a capacity shift due to parasitic current consumption, contribution of the SEI to overall lithium storage capacity, and self-discharge of the electrode during rest. The model also captures two different mechanisms for a halt in SEI growth: the depletion of solvent in the electrolyte, and the absence of lithium in the active phase.

References:

[1] Verma, Pallavi, Pascal Maire, and Petr Novák. ‘A Review of the Features and Analyses of the Solid Electrolyte Interphase in Li-Ion Batteries’. *Electrochimica Acta* 55, no. 22 (2010): 6332–41. 10.1016/j.electacta.2010.05.072.

[2] Manuel Landstorfer, Christoph Pohl, Ferran Brosa Planella, and Kawa Manmi. A Model for SEI-Growth Based on Non-Equilibrium Thermodynamics. 2025. 10.20347/WIAS.PREPRINT.3250.

[3] Landstorfer, Manuel. ‘A Discussion of the Cell Voltage during Discharge of an Intercalation Electrode for Various C-Rates Based on Non-Equilibrium Thermodynamics and Numerical Simulations’. *Journal of The Electrochemical Society* 167, no. 1 (2020): 013518. 10.1149/2.0182001JES.

Keywords: ModVal2026, li-ion batteries, modelling, SEI

Modeling and simulation of porous electrodes with phase separation based on non-equilibrium thermodynamics and homogenization theory

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Abstract

We present a mathematical modeling framework [1–3] for a porous intercalation electrode in which the active phase can undergo multiple phase transitions. The modeling is based on non-equilibrium thermodynamics and a multi-well free-energy function describing intercalated lithium in the active material. Special care is taken to ensure thermodynamically consistent boundary conditions for both the lithium intercalation reaction and lithium transport within the active phase.

The model is then formulated in a multiscale asymptotic setting, and leading-order equations are derived using periodic homogenization theory. The resulting coupled 3D+3D equation system is reduced to a macroscopic one-dimensional and a microscopic spherical one-dimensional geometry, yielding, in essence, a generalization of the DFN model [4] for materials exhibiting multiple phase transitions.

We present numerical simulations of full and partial charge–discharge cycles, which exhibit multiple voltage plateaus, hysteresis, and hysteretic loops, even under open-circuit voltage (OCV) conditions. The origins of these effects are explained in detail based on numerical solutions of the governing PDE system, leading to important conclusions regarding OCV functions with plateaus. For higher C-rates, we demonstrate how and why the plateaus steepen during cycling and predict a full-cell voltage spectrum as a function of state of charge and C-rate.

References

[1] M. Heida, M. Landstorfer, M. Liero, *SIAM Multiscale Modeling & Simulation*, 2024, **22**, 1068–1096.
[2] M. Landstorfer, M. Ohlberger, S. Rave, M. Tacke, *European Journal of Applied Mathematics*, 2023, **34**, 554–591
[3] M. Heida, M. Landstorfer, *WIAS Preprint 3251*, 2025
[4] T. Fuller, M. Doyle, J. Newman, *J. Electrochem. Soc.*, 1994, **141**, 1–9.
[5] M. Heida, M. Landstorfer, *in preparation*

Keywords: Porous Electrode, Homogenization, DFN, Phase Separation, Hysteresis

Coupled Transport, Poisson and gFBV Model for 1D Double Layer Description of RFB Electrode-Electrolyte Interface

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Abstract

Electrochemical reactions in redox flow batteries (RFBs) occur within a nanometric interfacial region where electric field, ion distributions, and charge-transfer kinetics are strongly coupled. Capturing the physics of this electrode–electrolyte interface is essential to build predictive models that can be consistently connected to larger-scale porous-electrode and cell-level descriptions [1]. In this work we present a physics-based continuum model of the electrochemical double layer for RFB operative conditions and for experimental setup simulations, obtained by coupling ionic transport (Nernst–Planck) with electrostatics (Poisson) and a generalized interfacial kinetic law. The charge-transfer boundary condition is formulated as a generalized Frumkin–Butler–Volmer (gFBV) relation [1], enabling reaction rates to depend on the local interfacial potential drop and on the near-surface concentrations shaped by double-layer charging. This framework provides spatially resolved profiles of potential, concentrations, and charge density across the interface (nm scale), and produces macroscopic observables such as current–potential (I–V) characteristics and differential capacitance as a function of electrode potential. Beyond steady-state predictions, the model is designed as a basis for frequency-domain analysis and for the development of a predictive, physics-based description of electrochemical impedance spectroscopy (EIS), a particularly sensitive technique to double-layer effects [2]. The proposed approach supports systematic parameter estimation and serves as a transferable interface module for multiscale RFB modeling.

References:
1. M. van Soestbergen, Russ. J. Electrochem., 48(2012), 6, 570-579
2. A. Lazanas et al., ACS Meas. Sci. Au, 3(2023), 3, 162-193

Acknowledgements: This work is funded by the Swiss State Secretariat for Education, Research and Innovation (SERI) and is part of the PREDICTOR MSCA Doctoral Network, funded by the European Union (Grant Agreement no. 101168943).

Keywords: ModVal2026, RFBs, Double Layer, Physics based Modelling, Solid-Liquid Interface

Qualitative Regime Behaviour in Reduced-Order Porous Electrode Models for Redox-flow Cells

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Abstract

Physics-based cell-scale models are a central component in enabling high-throughput screening of materials for redox-flow batteries through integrated modelling and experimentation. In this contribution, we explore the qualitative behaviour of minimal models and assess how modelling assumptions and operating conditions shape predicted electrochemical regimes.

Using simplified one-dimensional porous half-cell electrode formulations under galvanostatic operation, we analyse transitions between distinct limiting regimes and the emergence of characteristic reaction localization patterns within the electrode. A dimensional scaling perspective is adopted to identify the dominant processes controlling electrode utilization across operating conditions, providing a systematic framework to classify model behaviour and isolate performance bottlenecks.

We further examine the sensitivity of these minimal models to electrolyte transport assumptions, illustrating how alternative transport closures beyond the dilute limit can qualitatively affect predicted concentration, polarization and potential distributions. This highlights the role of transport modelling assumptions when assessing electrolyte composition and electroactive species properties at early screening stages.
Overall, this work shows how regime-aware, physically consistent reduced-order models can be used to identify performance-limiting mechanisms and inform material selection in redox-flow battery design.

Keywords: ModVal2026, redox-flow cells, dimensional analysis, physics based modelling

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Hooks, shoulders, knees and toes: Understanding bumps in LFP half-cell voltage curves through the composite phase-change model

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Abstract

Voltage curves measured from LiFePO4 (LFP) electrodes typically exhibit flat hysteretic plateaus, indicative of the phase changes that are known to occur in the material. On closer inspection, we find that there is often a ‘hook’, a small local maximum, on entry to the charging plateau. Moreover, there is often a ‘shoulder’, a small secondary plateau or inflection point, near the end of the charge. The large, flat plateaus have been modelled by lithiation-induced phase change [1] in a large number of interacting particles and modelled by the composite phase change model (CPM). However, computational expense limits the use of this model to a relatively small number of representative particles (~100) in comparison with typical numbers found in a real nanoparticulate LFP electrode (~10^{13}). This discrepancy in particle number can create artifacts which obscure the physics of the model, hampering interpretation. To combat this, we present the continuum composite phase-change model (CCPM), a natural extension in which we take the mathematical limit of infinitely many particles prior to numerical solution.

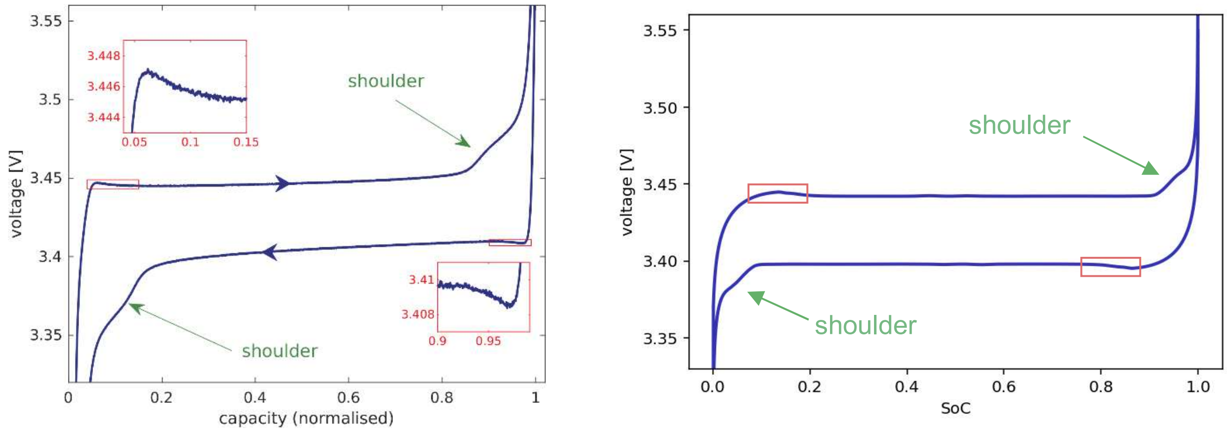

Fig. 1. Qualitative comparison between voltage curves of LFP half cells exhibiting flat plateaus, hooks and shoulders (left) and those predicted by the CCPM for phase-changing electrodes (right).

Armed with this new model, derived directly from the Cahn-Hilliard equation for phase separation in one particle and extended to the electrode scale, we explore its predictions for phase-change electrodes and compare them with LFP half-cell data. In doing so, we find that not only voltage plateaus but also hooks and shoulders are all natural predictions of the model, enabling detailed analysis through both numerical and asymptotic methods as to the

underlying causes. We arrive at intuitive explanations of both hooks and shoulders based on discrete quanta, or ‘packets’, of particles undergoing phase separation one after another, where the packet size is governed by the applied current.

References.

[1] Foster, J. M., Grudeva, Y., Korotkin, I., Dickinson, E. J., Offer, G., & Richardson, G. (2025). The Newman model for phase-change electrodes: physics-based hysteresis. Journal of The Electrochemical Society, 172(4), 040501.

Keywords: LFP; phase change; composite phase-change model

Optimal loading control accounting for cell-to-cell variability in parallel battery modules

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Abstract

The pace of development of lithium ion battery energy storage systems has placed increasing importance on battery usage optimization, which is essential for both safety and commercial viability. Large stationary battery packs are made up of many cells, often with parallel connections where individual branch currents and temperatures are not directly measured [1]. This makes it difficult for optimal loading and charging algorithms to maximise the performance of the pack, while protecting all the individual cells and extracting full value from the battery asset [2]. To address this challenge, we employ an electrothermal equivalent circuit model of parallel connected cells, integrated with a model predictive control framework to calculate optimal loading profiles for a battery system with four prismatic LFP cells connected in parallel. This approach enforces safety constraints on current, temperature, and voltage at the individual cell level within parallel groups, while determining the maximum possible power delivery of the pack. Crucially, the relationship between peak power capability and depth of discharge (DoD) has been characterised, as the modelling shows that operating with a lower depth of discharge enables a higher power delivery during discharge. This is achieved by avoiding current transients during periods of intense rebalancing in the parallel group, which typically occur in the low state of charge range [3]. This analysis is intended to help battery asset owners balance power and duration requirements for industrial energy storage systems.

Keywords: BatteryModelling, OptimalLoading, ParallelCells

References

[1] F. Alexander, S. Schaeffler, C. Kirst, F. Roehrer, S. Kücher, A. Durdel, M. Scheller and A. Jossen, “Modeling Inhomogeneities during Parallel-Connected Fast Charging of Lithium-Ion Battery Systems,” *Journal of The Electrochemical Society,* vol. 172, 2025.

[2] S. Fasolato, A. Allam, S. Onori and D. Raimondo, “Analyzing cell-to-cell heterogeneities and cell configurations in parallel-connected battery modules using physics-based modeling,” *Journal of Energy Storage,* vol. 129, 2025.

[3] A. Weng, M. Hamidreza, C. Wong, J. Siegel and A. Stefanopoulou, “Current Imbalance in Dissimilar Parallel-Connected Batteries and the Fate of Degradation Convergence,” *Journal of Dynamic Systems, Measurement, and Control,* vol. 146, 2024.

Kinetic Monte Carlo Modelling of Hydrogen Evolution and Iron Plating in Hybrid All-Iron Redox Flow Batteries

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Abstract

Hybrid All-Iron Redox Flow Batteries (IRFB) offer a viable pathway for long-duration energy storage. Nonetheless, the presence of parasitic hydrogen evolution reaction (HER) and irregular iron plating at the negative electrode remains a significant challenge, resulting in reduced Coulombic efficiency and a limitation on cycle stability.

The goal of this work is to understand the interactions between the processes on the interface of the negative electrode by combining a simulation model with experimental data. The HER can be catalyzed by iron on the electrode. The extent of this undesired effect depends on the structure of the iron precipitates. Modeling this interaction requires a simulation approach in which the reaction rates can be locally adapted to the surface conditions. Consequently, a simulation at the molecular level was implemented using the kinetic Monte Carlo method and a lattice gas model. To obtain a comprehensive view of the influences of individual parameters, we conducted experimental cyclic voltammetry (CV) at different temperatures, pH values, and iron concentrations to parameterize the model. The influence of mass transport limitations in electrolyte is minimized through the utilization of low current densities and a rotating disk electrode.

The basis for the combination of kMC and experimental CVs is a novel adapted sequence in the kMC loop, which calculates the continuous variation of global parameters such as electrolyte concentrations or anode potential in a computationally efficient manner. Furthermore, a concept was developed for simulating only the relevant processes on the electrode in kMC without having to represent the diffusion processes in the electrolyte, which further reduces computational cost. Together, these improvements enabled the parameterization of CV simulations exceeding 40 seconds in a substantial 3D BCC grid.

The model provides important insights into the interaction between iron plating and stripping and HER. It enables the separation of the current density in the CVs into the respective proportions of the reactions. It allows for a detailed investigation of the influences of binding energies between species and the influence of the morphology of iron deposition on HER. All considerations can be examined under different operating conditions, which allows knowledge-based optimization of the iron redox flow battery systems.

In conclusion, combining kMC with CV experiments clarifies the interaction of iron plating and hydrogen evolution, enabling reaction separation and guiding optimization of IRFBs.

Keywords: ModVal2026, kinetic Monte-Carlo method, cyclic voltammetry, hybrid Iron redox flow battery, metal plating, hydrogen evolution reaction

Reduced-Order Modeling of Polymer-Based Battery Electrodes

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Abstract

Organic redox polymers, particularly **TEMPO**–containing polymers, are being explored as cathode materials batteries due to their high-power density, flexibility and metal-free chemistry, yet their electrochemical behavior remains insufficiently characterized. This talk presents modeling and simulation efforts aimed at understanding the internal states of the organic polymer-based battery system.

We first present a dual-ion battery model based on the classical single-particle model with electrolyte (**SPMe**) and adapted for a **PTAm**-based polymer cathode. Validation against experimental data demonstrates that the model reproduces global voltage–capacity trends across the investigated operating range, indicating that the dominant transport and kinetic mechanisms are captured. Model deviations motivate further refinement, particularly through microstructure-informed transport parameters.

As a step toward microstructure-informed parameterization, we provide a preview of three-dimensional microstructural analysis on polymer-based composite electrodes, where the interplay between the polymer active phase, conductive additive, and binder governs coupled electronic and ionic transport. The results outline a pathway for integrating microstructural measurements with electrochemical models for emerging organic redox polymer batteries.

Keywords: polymer-based batteries; electrode microstructure; SPMe; dual-ion batteries

Optimal Control of a Half-Cell Equivalent Circuit Model for Li-ion Batteries with Applications to Fast Charging

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Abstract

With the proceeding emergence of electrical applications as electrical vehicles, smartphones, etc., the importance of mathematical models and simulations which adequately describe the behavior of batteries increases. In this context, also the question of suitable charging protocols rises, focusing on to reach a desired state of charge (SOC) in minimal time guaranteeing required cell-related quantities to stay in given bounds. Relevant examples for restrictions are comfort zones for cell temperature and total voltage (for safety reasons), anode potential (related to aging effects given by Lithium plating) and power input (given by further system requirements). This yields a crucial, however, due to different coupled physicochemical-thermal effects, nontrivial issue to solve. To tackle this in a reasonable manner, this work provides a half-cell equivalent circuit model coupled with a 0D-thermal model to simulate required cell outputs. Based on this, a gradient-based optimization framework is presented to elaborate promising charging protocols for Li-ion batteries in a numerically efficient way.

Here, the mathematical model is used to describe the single electrodes and temperature as satisfactory compromise between accuracy and computational complexity. The SOC is calculated via Coulomb counting. Further, due to the therein defined system of ordinary differential equations, the mentioned optimization task is represented as a so-called optimal control problem with state inequality and equality constraints. Discretizing the model in the time domain results in a high-dimensional system to optimize. For this, a gradient-based optimization method is used since it allows to reach the optimum in a more efficient way compared to gradient-free methods. In this work, the sensitivities of the outputs with respect to current and final time are calculated recursively. The mentioned procedure leads to a further substantial speed-up of the optimization routine compared to typically used finite difference approximations, in these cases by several powers of 10. The derived optimized load profiles are compared to different, typically used charging protocols. Finally, simulatively obtained results are complemented by validation with a commercial LFP pouch cell.

Keywords: ModVal2026, Li-ion cell, optimal control, half-cell ECM, fast charging, efficient gradient calculation

Bridging Cell and System Scales: Coupled Electrochemical and Thermal Simulation of Batteries with Silicon-Dominant Anodes

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Abstract

Physics-based battery simulations provide profound insights into electrochemical processes and offer predictive capabilities due to its rigorous physical foundations. However, such simulations are typically limited to the analysis of single cells, neglecting the influence of the operational environment, including neighboring cells, thermal management systems, and other external factors. In practical applications, cells are embedded in complex systems where these interactions play a crucial role in overall performance and safety.

To address this gap, we present a multi-scale simulation approach that integrates detailed cell-level modeling with system-level dynamics. At the system level, we employ MATLAB/Simulink to capture the thermal and electrical behavior of battery systems under realistic operational conditions. For the cell-scale simulation, we utilize the Battery and Electrochemistry Simulation Tool (BEST) developed by Fraunhofer ITWM, which enables highly customized modeling of cell behavior by considering the physical properties of constituent materials and detailed electrode geometry. The underlying model is an extended pseudo-2d Doyle-Fuller-Newman (DFN) framework that couples electrochemical and thermal phenomena.

A notable feature of our approach is the extension of the cell model to incorporate the voltage hysteresis characteristic of silicon anodes, implemented based on the empirical methodology proposed by Plett. This enhancement is particularly relevant for next-generation lithium-ion batteries, where silicon-based electrodes are increasingly employed to achieve higher energy densities.

The integration of BEST and Simulink is achieved via the Functional Mock-up Interface (FMI) standard, enabling efficient co-simulation of cell and system-level models. This direct coupling facilitates the investigation of complex scenarios, such as dynamic electrical loads and temperature gradients within the cell stack.

In this contribution, we detail the technical realization of the coupling between BEST and Simulink, describe the implementation of the hysteresis extension for silicon anodes, and demonstrate the capabilities of the approach through selected case studies.

Keywords: DFN model, silicon voltage hysteresis, multiscale battery simulation

Optimization of ion mobility in Li-ion batteries by metal fibers

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Abstract

The mobility of Li-ions in the electrolyte is a limiting factor for battery design. Recently, Wang et. al. proposed that Li-ion mobility can be improved by embedding metallic fibers that serve as current collector [1]. They attribute this improvement to the breaking of Li-ion-solvent complex within the Helmholtz layer adjacent to the metal surface.

This raises the question of optimal fiber density as improvement of ion mobility should overcompensate the drawback of additional inert material. As experimental optimization is expensive and time-consuming, we have developed a predictive macroscopic, electrochemical model of the battery cell taking the improved surface transport along the fibers into account. Ion transport along the metal surface is modeled by adsorption and surface diffusion.

Rigorous 3D simulations of particle packing and embedded fibers are far too expensive for optimization purposes which should identify fiber density, fiber thickness and cell thickness under the constraint of a required power density.

Instead, we investigate a representative cylindrical volume of the cell with a single metal fiber embedded in axial direction (Fig 1). Ion transport in the electrolyte is modelled as a homogeneous field using effective transport parameters which take the tortuosity of the particle packing into account. As diffusion is a linear transport operator, the parameters can be obtained by mathematical homogenization. The particles are also modelled by a homogeneous field using an approach developed previously [2].

The model allows to account for effective radial and axial transport in the packing, transport limitations within the particles and improved transport along the metal surface. For a given geometry of the particles and transport parameters within particle and electrolyte optimal fiber diameter, cell thickness and number density of the fibers can be calculated under the constraint of a required power density.

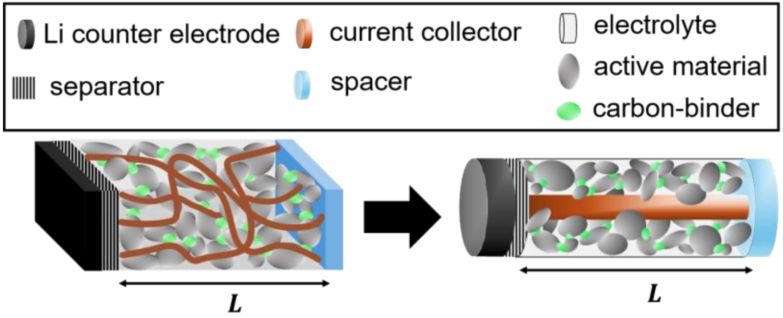

Figure 1. Left: Li-ion half cell with metal fiber network as current collector. Right: Representative cylindrical volume of the half cell.

[1] Wang, Yuanzhen; Aubermann, Florian; Spatz, Joachim P. (2025): Enhanced Ion Mobility in Helmholtz Layer Enabling Ultrathick Electrodes. In: *ACS nano* 19 (18), S. 17917–17928. DOI: 10.1021/acsnano.5c04343

[2] G. Lombardo, Y. Wang, C. Stockinger, J.P. Spatz, U. Nieken, A Particle-Based Model Reduction for Lithium-Ion Batteries, J. Electrochem. Soc. 172 (2025). https://doi.org/10.1149/1945-7111/add910

Keywords: ModVal2026, Li-ion-battery, enhanced Li-ion mobility, macroscopic model, design of metal fiber network

Impedance of battery electrolytes: an analytical approach

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Abstract

Electrochemical impedance spectroscopy (EIS) is widely used to probe physical processes within electrochemical systems and, when coupled with a physics-based model, enables non-invasive parametrisation in the frequency domain. In the case of battery electrolytes, the impedance spectrum of a symmetric cell can be used to find transport properties. Commonly, ionic conductivity is recovered from high-frequency spectra.

Electrolyte impedance is most simply modelled by a finite Warburg element. This type of description intrinsically assumes that the system is at periodic steady state, a condition required to correctly calculate impedance [1]. However, when working with time-series data, transient decay timescales must be carefully accounted for to avoid erroneous results. In this work, we revisit the volume-averaged electrolyte transport model originally developed by Newman and Chapman [2] and later non-dimensionalised by Liu and Monroe [3], where ion movement is attributed to diffusion and Faradaic convection. Then, without invoking the steady-state approximation, we solve for impedance analytically using asymptotic analysis and Laplace transform methods - an approach novel for this application.

Retaining transient behaviour allow us to derive a criterion for the number of ac periods required to reach a stationary system response, which is shown to increase with frequency. This result challenges the conventional practice of discarding a fixed number of periods regardless of frequency. Furthermore, extending the analysis beyond leading order allows us to probe the effects of Faradaic convection on impedance.

References

[1] Mark E. Orazem and Bernard Tribollet. “Electrochemical Impedance Spectroscopy”. In: Electrochemical Impedance Spectroscopy (Feb. 2008), pp. 1–523. doi: 10.1002/9780470381588.
[2] John Newman and Thomas W. Chapman. “Restricted diffusion in binary solutions”. In: AIChE Journal 19.2 (Mar. 1973), pp. 343–348. issn:1547-5905. doi: 10.1002/AIC.690190220.
[3] Jing Liu and Charles W. Monroe. “Solute-volume effects in electrolyte transport”. In: Electrochimica Acta 135 (2014). issn: 00134686. doi:10.1016/j.electacta.2014.05.009.

Keywords: ModVal2026, EIS, electrolytes, analytical approaches, transient decay

A Time-Dependent 0D Model of Redox Targeting-Based Flow Batteries with Two-Step Electron-Transfer Reactions

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Abstract

Redox flow batteries, in comparison to classical battery concepts, enable independent scaling of power and capacity but face energy density limitations due to the solubility constraints of redox-active species in the electrolyte. Redox targeting-based flow batteries with a solid depot circumvent this limitation by relocating energy storage to high-capacity solid materials within the tank, with dissolved mediators solely facilitating the charge transport between the cell and the solid material. This configuration consequently introduces additional reaction pathways - particularly in multi-step electron transfer reactions - and coupled transport processes, increasing system complexity.

This study implements a time-dependent 0D model of a single-molecule redox targeting-based flow battery following [1]. The model treats the tank and cell as ideally mixed reactors connected through electrolyte flow rate. It models reactions in both cell and tank using two successive electron transfer steps, accounting for varying redox potentials in these partial reactions. Cell reaction kinetics are modeled using Butler-Volmer equations, while tank reactions are described via Mixed Potential Theory [2]. The numerical simulation then enables a discrete analysis of the contributions from various system components and individual electron transfer steps to voltage and capacity losses.

The model is employed to examine how the interplay between multi-step electron transfer reactions and operational parameters influences battery efficiency and tank utilization. Specifically, it analyzes the impact of redox potential separation in two-step reactions on voltage losses and achievable state of charge in the tank and the cell. The findings aim to establish straightforward design and operational guidelines for future redox-mediated flow batteries with multi-step electron transfers and provide a foundation for more sophisticated, spatially resolved models.

Keywords: Long-term energy storage, numerical multi-physics simulation, system optimization, battery efficiency, single-molecule redox-targeting process

References:

1. Shu, G.; Cao, H.; Yan, Z.; Wang, W.; Tian, H. *Energy Convers Manag* **2026**, *347*, 120527.
2. Matteucci, N. J.; Mallia, C. T.; Neyhouse, B. J.; Brushett, F. R. *J Electrochem Soc* **2025**, *172*, 070539.

Model-based quantification of specific energy and thickness change of lithium-ions cells with silicon-graphite negative blend electrodes

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Abstract

Combining silicon and graphite in a blend negative electrode for lithium-ion batteries allows for the utilization of both the high specific capacity of silicon and the long cycle life of graphite [1]. The present study employs a multiphysics pseudo-three-dimensional (P3D) model to investigate the electrochemical and mechanical behavior of silicon-graphite blend electrodes. The model is based on a coupled thermal-electrochemical-mechanical framework and integrates fictitious silicon particles into an existing 350 mAh lithium-ion pouch cell, which features an LCO/NCA positive electrode and a graphite negative electrode. This reference cell has been fully parameterized by Carelli et al. [2]. Key material parameters, such as the lithium diffusion coefficient in silicon, were obtained from the literature, and a novel thermodynamic approach was introduced to capture the voltage hysteresis of silicon. Model validation was conducted using experimental silicon half-cell data against Li/Li$^+$. Subsequent simulations explored the effects of negative electrode thickness, silicon volume fraction, and particle size on electrochemical performance and mechanical expansion. The results show that thinner negative electrodes promote a higher degree of lithiation due to enhanced electrolyte-active material contact, although this also leads to increased mechanical stresses, despite an improvement in gravimetric energy density. The specific energy exhibits a distinct maximum that shifts toward lower electrode thickness as silicon volume fraction increase. Notably, the electrode thickness that achieves maximum mechanical expansion exceeds that of the specific energy optimum, underscoring a trade-off between energy maximization and mechanical stability. Variations in particle size demonstrated that smaller silicon particles achieve higher degrees of lithiation due to their larger surface-to-volume ratio, while larger particles induce pronounced mechanical stress. Furthermore, microscale lithium stoichiometry gradients within the graphite and silicon phases were visualized, revealing nearly gradient-free lithiation behavior in silicon for smaller particle sizes.

[1] P. Lv, H. Zhao, C. Gao, T. Zhang, and X. Liu, Electrochim. Acta 152, 345–351 (2015), doi: 10.1016/j.electacta.2014.11.149.
[2] S. Carelli, M. Quarti, M. C. Yagci, and W. G. Bessler, J. Electrochem. Soc. 166, 2990–3003 (2019), doi: 10.1149/2.0301913jes.

Keywords: Lithium-ion battery, silicon-graphite blend electrode, pseudo-three-dimensional (P3D) model, voltage hysteresis

LIBquiv: An open-source MATLAB class for time-domain simulation of battery equivalent circuit models

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Abstract

Lithium-ion battery technology represents the most important electrical energy storage solution today, supporting applications ranging from portable electronics to grid-scale storage. Mathematical modeling and simulation are essential for the development of modern battery management systems. Equivalent circuit models (ECMs) remain the preferred choice for practical applications due to their computational efficiency and ease of parameterization [1]. Despite their widespread use, there is a notable scarcity of open-source software dedicated to time-domain ECM simulations, often forcing researchers to rely on custom implementations or commercial alternatives.

This work introduces LIBquiv, an open-source MATLAB class designed for the time-domain simulation of battery ECMs, characterized by its flexibility and ease of use. The tool is capable of simulating a wide spectrum of model architectures, ranging from simple empirical circuits to complex, physics-informed ECMs. This includes models that incorporate specific electrode resistances, aging-sensitive parameters, and thermal equivalent circuits to account for the significant impact of temperature on battery performance and longevity.

Mathematically, LIBquiv handles the time-dependent nonlinear differential-algebraic equation systems inherent to ECMs through an object-oriented framework and solves them efficiently by using MATLAB's ode23t solver. This architecture allows users to operate the digital battery model in a manner analogous to experimental laboratory procedures. Simple commands allow constant-current, constant-voltage, or constant-power simulations, complete with customizable cut-off criteria. The flexibility of LIBquiv is demonstrated in use cases of previous studies involving various cell formats and chemistries, such as large-format and prismatic lithium iron phosphate cells as well as cylindrical Panasonic cells [2]. In the present contribution we make the code available open source. Full parameter sets and validated examples are provided with the code to support the scientific community in the simulation, optimization, and diagnosis of lithium-ion systems.

[1] W. G. Bessler and M. Dubarry, in Julia Kowal and Dirk Uwe Sauer (Editors), "Simulation models of secondary batteries", Elsevier (2026)
[2] P. O. Mmeka, M. Dubarry, W. G. Bessler, J. Electrochem. Soc. 172, 080538 (2025), https://doi.org/10.1149/1945-7111/adf9cb .

Keywords: Lithium-ion batteries, equivalent circuit model, time-domain simulation, MATLAB, open-source

Homogenization of LIBs: a fast model for state-of-charge in-line monitoring

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Abstract

Lithium-ion batteries (LiBs) offer high energy density, low self-discharge, and decreasing production costs, but their performance and lifetime are often limited by local inhomogeneities, including non-uniform current distribution and concentration gradients. Electrode morphology strongly influences these effects, yet it is frequently oversimplified in conventional models because resolving realistic pore-scale geometries is computationally expensive.

This work builds a rigorous link between microscopic transport physics and macroscopic battery-scale modelling by applying homogenization via multiple-scale expansion to a lithium-ion cell [1]. Starting from pore-scale governing equations for mass and charge transport in the electrolyte and solid phases, we derive an upscaled macroscopic formulation in which the complex microstructure is replaced by effective transport properties. The approach exploits scale separation between a characteristic macroscopic length L (electrode/cell scale) and a microscopic length l (particle/pore scale). Under the common condition $L \gg l$, the homogenized model is significantly faster than pore-resolved simulations while introducing a controlled approximation error of order $\mathcal{O}(l/L)$.

The equations are cast in dimensionless form to identify relevant Péclet and Damköhler regimes and to define conditions for homogenization. Effective parameters are then obtained by solving closure problems on a periodic unit cell representative of the electrode morphology, yielding effective diffusivity and electrical conductivity for both liquid and solid phases and naturally accounting for porosity and tortuosity. For graphitic anodes, where particle anisotropy can affect transport pathways, the microstructure can be generated using flattened ellipsoidal particles informed by experimental particle size distributions and SEM-derived aspect ratios, providing a more realistic alternative to spherical particles.

The resulting homogenized model is implemented and verified against a fully resolved 4D pore-scale simulation on the corresponding reconstructed microstructure. The homogenized formulation reproduces the main pore-scale trends with substantially reduced computational time and resources, enabling rapid parametric studies of morphology and operating conditions. Overall, homogenization provides a fast yet predictive framework for LIB simulations, supporting BMS implementation and fast in-line prediction for state-of-charge monitoring.

[1] Arunachalam, H., Onori, S., Battiato, I., **(2015)**, *On Veracity of Macroscopic Lithium-Ion Battery Models. J. Electrochem. Soc.*, 162, A1940

Assessing the Limitations of 1D Models in Large-Format Batteries: A Comparative P2D and P4D Study on Aspect Ratio Effects

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Abstract

As the demand for large-format lithium-ion batteries (LIBs) grows, particularly for electric vehicle applications, understanding internal inhomogeneities becomes critical for ensuring safety and performance. While the Pseudo-two-dimensional (P2D) model is widely used for battery simulation, its one-dimensional nature inherently fails to capture lateral (in-plane) gradients in electrochemical and thermal variables. This study investigates the limitations of 1D models by comparing them with an efficient, non-iterative Pseudo-four-dimensional (P4D) framework across various cell aspect ratios.

We developed a high-fidelity P4D solver that accounts for three-dimensional transport and heat generation, validated against FEM-based simulations. To quantify the internal non-uniformity, a Scaled Uniformity Index (UI) was employed to analyze spatial distributions of lithium concentration, overpotential, and temperature. Our results demonstrate that as the cell aspect ratio increases—keeping the total area constant—in-plane inhomogeneities significantly intensify, leading to localized deviations in voltage behavior and increased risks of lithium plating that are completely overlooked by the P2D model. The findings emphasize the necessity of 3D modeling for the accurate design and validation of large-format cells, providing a quantitative threshold where 1D approximations become insufficient.

Keywords: ModVal2026, Large-format Lithium-ion Batteries, P4D Modeling, In-plane Inhomogeneity

Electrolyte Motion in Lithium-ion Batteries - A Multiscale Modelling Framework

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Abstract

Electrolyte motion within cylindrical lithium-ion cells is increasingly recognized as a source of capacity loss[1], yet the physical drivers behind this motion are difficult to disentangle experimentally because multiple coupled mechanisms act simultaneously during operation. To address this, we develop a multiphysics and multiscale modelling framework that includes electrolyte motion resulting from multiple electrochemical and mechanical sources.

The framework extends previous modelling work, which concentrated on electrode expansion as the source of electrolyte motion[2], by incorporating additional mechanisms that are expected under realistic cell conditions, namely elastic stack compression and concentration-dependent electrolyte volume changes. Mechanical behavior is represented in a way that allows local variations in stack pressure, influencing porosity and in turn modifies electrochemical transport pathways. The electrolyte phase is modeled with density and viscosity permitted to vary with salt concentration and temperature, enabling feedback between operating conditions, local transport properties, and flow response. To obtain accurate values for the electrode permeability, which is an important model parameter for the flow, we perform mesoscale analysis of reconstructed electrode microstructures from X-ray computed tomography.

Using this framework, we examine how different combinations of mechanical boundary conditions and electrolyte property couplings influence the details of the electrolyte flow pattern. The simulations indicate that electrolyte motion can arise even in the absence of strong mechanical confinement, while imposed stack pressure can amplify flow and introduce regional differences in flow behavior. The results highlight that property–transport couplings and microstructure-sensitive permeability can substantially influence predicted flow pathways, suggesting that electrolyte motion is not governed by a single mechanism but by interacting effects that depend on both design and operating state.

[1] Solchenbach, S. et al. Electrolyte motion induced salt inhomogeneity – a novel aging mechanism in large-format lithium-ion cells. Energy Environ. Sci. 17, 7294–7317.
[2] Boveleth, L., Okraschevski, M., Danner, T. & Latz, A. A 3D battery model incorporating Si particle expansion induced electrolyte motion. Journal of Energy Storage 141, 119206.

Keywords: ModVal2026, lithium-ion batteries, electrolyte motion induced salt inhomogeneity, P3D electrochemical simulation.

Investigation of Effective Transport Parameters of Lithium-Ion Cells Using a Hybrid Simulation Model

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Abstract

The performance and aging behavior of a lithium-ion battery are strongly influenced by the internal multiphysical processes in combination with external factors such as thermal management systems. However, the internal processes, their quantification, and their changes during operation and aging are not easily accessible and require a high level of characterization effort. To gain insights into these processes, simulation models have established themselves as a proven and useful tool for elucidating the complex interactions between charge, heat and mass transport as well as electrochemical reactions. By combining experimental measurement data with simulation models, internal physical transport parameters can be evaluated and determined. However, such inverse parameterizations require in-depth knowledge of the interactions between internal cell parameters and integral cell behavior.

In this work, a model was developed that consists of a combination of an equivalent circuit model and a physical pseudo-2D model based on the Doyle-Fuller-Newman (DFN) approach. This model is used to predict impedance spectra based on multiphysical processes and to systematically analyze the underlying parameters. By comparing the impedance spectra from the simulation with experimental data, the physical parameters that determine the overall behavior of the cell can be identified. This inverse parameterization approach was accelerated by implementing a least-squares optimization that fits the simulated impedance spectra to an experimental data set by automatically optimizing the values of the physical parameters. In addition, the voltage behavior of the cell is analyzed to gain further information about parameters that are sensitive in the time domain.

A challenging task when applying a DFN modeling approach in combination with an optimization algorithm is to identify the value range and the interaction of the key effective transport parameters that are influenced by the microstructure of an electrode. Based on previous work on the sensitivity of each model parameter and the comparison with a heterogeneous 3D microstructure model, the range of effective transport parameters can be narrowed down. The developed 3D microstructure simulation model is then used to analyze the impedance and voltage behavior and to derive important effective transport parameters such as the tortuosity of the porous electrodes.

Keywords: Lithium-Ion Batteries, Multiphysical Modelling, Inverse Parameterization, Electrochemical Impedance Spectroscopy

Understanding the performance of LMFP/NMC blend cathodes with the help of simulation

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Abstract

Battery cells with blended electrode materials are gaining importance as they allow to increase energy density without compromising power density. A common example is anodes made from graphite and silicon blends, which significantly increase energy density while achieving a long cycle life. For cathodes, blends of $LiMn_xFe_{1-x}PO_4$ (LMFP) are successfully used. LMFP is a promising candidate to achieve higher energy densities at similar safety levels compared to LFP. However, its low electronic conductivity and sluggish Li-ion diffusion kinetics are major challenges for rate capability. Due to its comparable potential window, blends with NMC are often used to overcome these difficulties.

Blending of materials increases complexity, and depending on the operating conditions such as temperature, SOC, or C-rate, both cathode materials can impose limitations on cell performance. To better understand the interplay between these materials, a commercial 26700 cylindrical cell with an LMFP/NMC blended cathode is experimentally characterized with the goal of creating a virtual twin based on the P2D approach in the system modelling platform AVL CRUISE^{TM} M. In this study, the established approach of a homogenized model with a single effective cathode material is compared with a heterogeneous electrode model that treats both materials separately. The two models are parameterized and compared to illustrate the potential and limitations of the homogenized modeling approach.

An experimental procedure is tailored to identify all relevant model parameters with a minimum amount of effort and time. This includes various quasi-steady, dynamic load profiles and the measurement of impedance spectra at different SOCs and temperatures. The obtained data are fed into a semi-automated parameterization workflow to balance the electrodes and to obtain kinetic and transport properties.

At room temperature, both models show good agreement with the experimental voltage and temperature response, although the homogeneous model loses accuracy at higher C-rates. At reduced temperatures, the gap between measurement and simulation widens. In the experiments, capacity declines at moderate C-rates, which is not well predicted with the homogeneous electrode model. In contrast, using the heterogeneous electrode model, the observed reduced cell capacity can be reproduced and attributed to the individual materials. The sluggish diffusion in LMFP limits charging capacity, while the rapid decline in NMC kinetics at lower temperatures restricts discharging capacity. In addition, it is demonstrated that the use of two distinct materials is essential for reproducing impedance spectra.

Keywords: Li-ion battery cell, LMFP, blended electrode, P2D model

Thermodynamically consistent modeling of ion exchange membranes in multi-ionic environments

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Ion exchange membranes (IEMs) have enormous potential to improve a range of electrochemical technologies, including water desalination, fuel cells and batteries. E.g., in zinc-manganese batteries, the crossover of zincate degrades the manganese electrode by formation of poorly soluble phases such as hetaerolite; in zinc-air batteries the zincate can clog the air electrode through precipitation. Thus, suppressing parasitic crossover while imposing minimal hindrance towards functionally relevant transport can significantly extend battery lifetime. [1,2]

Since common membrane models are usually limited in their applicability or predictive value for highly concentrated multi-ionic environments, we formulate a more broadly applicable, thermodynamically consistent multiscale framework. This framework combines exclusion, single-site occupation and mean-field interactions along the polymer chain, consolidating central ideas of established membrane models into a unified free-energy description. [3,4,5]

The resulting model not only matches the experimental data well even at high ion concentrations, but also provides detailed insight into the underlying mechanisms and recovers key findings of several common membrane models as limiting cases. Incorporation of this model into a cell-scale battery simulation enables theory-guided membrane optimization for enhanced aqueous battery lifetime and efficiency.

[1] Fan, H. et al.; Advancing ion-exchange membranes to ion-selective membranes; *Frontiers of Environmental Science & Engineering* (2021, Vol. 17)
[2] Tsehaye, M.T. et al.; Membranes for zinc-air batteries: Recent progress, challenges and perspectives; *Journal of Power Sources* (2020, Vol. 457)
[3] Bowen, W.R. et al.; Modelling the performance of membrane nanofiltration; *Chemical Engineering Science* (2002, Vol. 57/7)
[4] Ion Activity Coefficients in Ion Exchange Polymers: Applicability of Manning's Counterion Condensation Theory; *Macromolecules* (2015, Vol. 48/21)
[5] Freger, V.; Ion partitioning and permeation in charged low-T* membranes; *Advances in Colloid and Interface Science* (2020, Vol. 277)

Keywords: ModVal2026, Ion exchange membranes, partitioning, permeability, aqueous batteries, theory-guided membrane optimization

Parametrization of phase-separating materials in the Newman model

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Abstract

Li-ion battery modeling took a leap forward thanks to the famous Doyle-Fuller-Newman (DFN) model designed in the early 90's. The first model formulation used the simple Fick's law for transport in the solid phase, whereas a large number of current commercial insertion materials actually display a phase transition behaviour. This simplification has long been overlooked in the battery community, as the model with the Fick approximation correctly predicts the cell potential during battery cycling in a large range of charge/discharge rates. However, it has been more recently observed that several macroscopic phenomena, such as voltage hysteresis, macroscopic lithiation heterogeneities, or spurious voltage relaxation, cannot be captured by the Fickian DFN model [1-3]. The phase-field dynamics also strongly shifts the predicted chargeability limits of graphite anodes, a major modeling challenge for industrial applications. The integration of a phase-field dynamics in the DFN model not only increases the numerical cost, but it also raises questions about its parametrization as the chemical potential of electrode materials with a phase separation is not experimentally accessible. In the present work, we present a formulation of the DFN model with phase-field dynamics based on the Cahn-Hilliard equation. The model is applied to a PBA positive electrode in a Na-ion battery and to a graphite negative electrode in a Li-ion battery. The phase-field parameters for the PBA electrode are directly obtained from ab-initio atomistic computations, thereby bridging the modeling gap between the crystalline scale and the electrode scale [4]. The phase-field parameters for the graphite electrode are deduced both from fundamental models and from electrochemical signatures of the phase-field dynamics in experimental characterization.

Keywords: Newman model, phase separation, Cahn-Hilliard equation, insertion materials

References:
[1] J. M. Foster *et al* 2025 *J. Electrochem. Soc.* **172** 040501
[2] T. Katrašnik *et al* 2023 *Advanced materials* **35**(31) 221093
[3] A. Vasileiadis *et al* 2018 *Advanced Functional Materials* **28**(16) 1705992
[4] Y-C. Yang *et al* 2026 submitted to *PRX energy*

Comparison of SEI-Growth Models for Lithium-Ion Batteries

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Abstract

SEI growth is a dominant contributor to degradation in lithium-ion batteries[1]. Investigations aimed at gaining a better understanding of SEI growth have resulted in numerous physico-chemical SEI-growth models proposed in literature, each relying on different limiting factors for the occurring side reaction[2]. In this work, we compare several established SEI-growth models available in the open-source battery modeling framework PyBaMM[3]. The models differ in their treatment of reaction kinetics, transport limitations, and dependencies on temperature and electrode potential. We analyze how well each model can be fitted to a three-year calendar-aging dataset of an LFP/C cell[4] using a nonlinear optimization algorithm. We compare the simulated and experimentally observed capacity fade across multiple aging conditions, such as resting temperature and state of charge. Preliminary results reveal differences in the ability of the various models to reproduce the measured calendar-aging behavior. Our study highlights the impact of different SEI-model assumptions and provides guidance on the selection of suitable SEI-growth models for calendar-aging simulations.

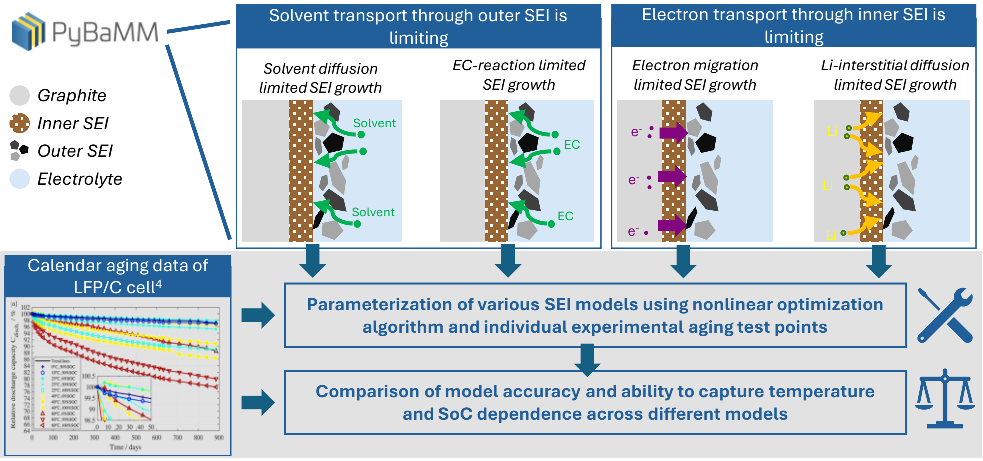

Figure 1: Overview of the SEI modeling approaches and workflow used for comparison.

Keywords: ModVal2026, SEI growth, aging model, LFP/C, calendar aging

References:

[1] Alexander Karger *et al* 2024 *J. Electrochem. Soc.* **171** DOI: 090512 10.1149/1945-7111/ad76da
[2] F. Single *et al* 2018 ChemSusChem **11.12** DOI: 10.1002/cssc.201800077
[3] V. Sulzer *et al* 2021 *J. open research software* **9** 1 DOI: 10.5334/jors.309
[4] M. Naumann *et al* 2018 *J. Power Sources* **17** (153-169) DOI: 10.1016/j.est.2018.01.019

Solid Electrolyte Interphase Model Based on Non-equilibrium Thermodynamics

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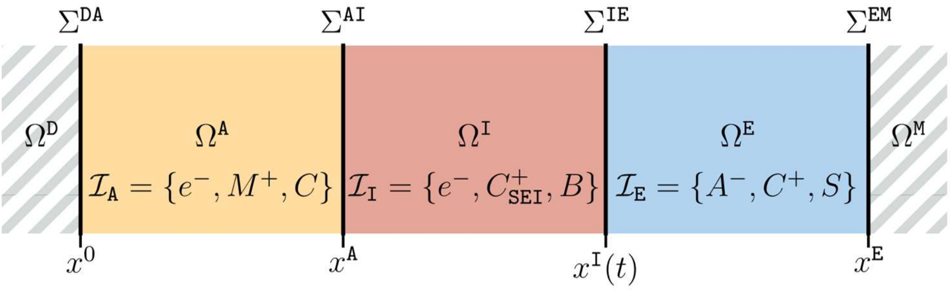
Abstract:

The solid electrolyte interphase (SEI) is a critical component in lithium-ion batteries, responsible for both initial capacity loss and ongoing degradation throughout the battery's lifetime. Understanding SEI formation and growth is essential for reducing manufacturing costs (which account for 20–30% of production expenses) and extending battery life.

We present a novel continuum-level model for SEI growth based on non-equilibrium thermodynamics at the microscale. The model comprises three coupled phases (electrode, SEI, and electrolyte) with thermodynamically derived interface conditions. The framework includes two competing reactions at the SEI-electrolyte interface (SEI formation and lithium intercalation) and systematically captures the coupling between electrochemical reactions, transport phenomena, and moving boundary dynamics.

Microscale 1D numerical results under OCV conditions demonstrate how formation reaction rates and electrolyte reservoir size influence SEI growth kinetics. The model captures self-discharge behaviour during rest periods and reveals how solvent consumption limits long-term SEI growth. We also present an upscaling framework using asymptotic homogenization to derive macroscale equations, exploiting the length scale separation between microscale structure and cell-scale to enable computationally efficient battery-scale simulations while maintaining thermodynamic consistency.



Schematic of the three-phase model showing electrode ($\Omega^{\mathtt{A}}$), SEI ($\Omega^{\mathtt{I}}$), and electrolyte ($\Omega^{\mathtt{E}}$) domains with thermodynamically consistent interface conditions. The SEI-electrolyte interface $\Sigma^{\mathtt{IE}}$ evolves as a moving boundary.

Probing simulation-based inference for credible battery model parameter estimation from impedance data

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Abstract

Electrochemical battery models like the Doyle-Fuller-Newman (DFN) model are increasingly being employed for tasks such as model predictive control during fast charging or model-based cell design. However, their parametrization poses a significant bottleneck for their widespread adoption. The DFN model contains numerous cell-specific parameters, whose determination usually involves time-consuming lab work. Data-driven parameter estimation has therefore emerged as a key factor in battery research.

Hitherto, fitting model parameters to voltage data via global optimization has arguably been the standard approach in literature. Recently, impedance has shown promise as a more efficient data source, due to its separation of processes on different time scales. Additionally, shortcomings of global optimization, e.g., missing information about identifiability, have motivated Bayesian approaches for parameter estimation.

We employ neural posterior estimation, a simulation-based inference algorithm, and compare its performance to particle swarm optimization, a metaheuristic global optimization approach commonly used in literature, for the estimation of 17 model parameters from synthetic impedance data with known ground truth parameter values. We use the inferred posterior for an analysis of compensation mechanisms among the parameters of the model and investigate the estimation quality when the prior distribution is sequentially updated.

Our findings suggest that Bayesian inference is more efficient and reliable for battery model parameter estimation while also enabling insightful analysis of the obtained results. Correlations among DFN model parameters are presented and discussed in the context of parametric identifiability for non-invasive parametrization from impedance data.

This work hence contributes to the advancement of reliable data-driven parametrization workflows for electrochemical battery models, thereby facilitating model-based research and development across academia and industry.

Keywords: ModVal2026, Bayesian inference, neural posterior estimation, lithium-ion battery, Doyle-Fuller-Newman model, electrochemical impedance spectroscopy

Calibrating P2D Battery Models with Gradient-based Optimization: From Single-Objective Sensitivity-Based Grouping to Multi-Objective Game-Theoretic Strategies

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Abstract

This work presents a systematic workflow for the calibration of pseudo-two-dimensional (P2D) battery models. The method addresses core challenges in parameter identification, including disparate parameter scales, low identifiability, and conflicting objectives across different operating regimes. The framework is built upon efficient adjoint-based gradient optimization, which provides accurate and scalable sensitivity calculations.

Calibration proceeds sequentially. First, equilibrium parameters are resolved using a simplified cell balancing approach. Second, a sensitivity-based parameter grouping strategy is applied to kinetic parameters, targeting high-rate discharge data. Finally, when a single parameter set fails to generalize across operating conditions, a game-theoretic Nash equilibrium algorithm is employed to reconcile multi-rate data as a multi-objective problem, yielding either a unique consensus or an ensemble of plausible solutions. This staged process inherently provides a form of uncertainty quantification through the analysis of parameter variability.

The complete workflow is demonstrated and validated using experimental data from a commercial lithium-ion cell.

Keywords: Battery modeling, Parameter identification, Sensitivity analysis, Adjoint-based optimization, Game-theoretic calibration

Analytical Approximations of Porous Electrode Theory for Reaction-limited Batteries

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Abstract

Physics-based models of lithium-ion batteries, such as the Doyle-Fuller-Newman (DFN) framework, provide critical insights into internal electrochemical states but are often computationally prohibitive for real-time control and large-scale optimization. This work presents practical approximations for reaction-limited, solid-solution electrodes, bridging the gap between high-fidelity simulations and reduced-order models. By exploiting the separation of timescales between fast intra-particle transport and slower discharge processes, and utilizing special functional forms of intercalation kinetics supported by experimental data, we derive approximations for key electrochemical variables. We introduce a set of dimensionless groups—specifically the reaction (Da_p), electrolyte transport (Da), and wiring (Da_w) Damköhler numbers—that govern the competition between reaction kinetics, ionic diffusion, and electronic conduction. The analytical predictions for galvanostatic discharge, chronoamperometry, and electrochemical impedance spectroscopy (EIS) are validated against full numerical simulations for a commercially relevant NMC half-cell. The model demonstrates excellent agreement under moderate C-rates and provides a physically interpretable framework for accelerated cell design and battery state estimation.

Keywords: ModVal2026, lithium battery, digital twin, porous electrode theory

Multi-Disciplinary Design Optimization of Li-ion Batteries: Coupling Electrochemical, Mechanical, and Thermal Performance

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Abstract

Increasing electrode layer thickness and thereby the active mass portion is a primary strategy for maximizing the energy density of Lithium-ion batteries (LIBs). However, this geometric modification introduces critical trade-offs, particularly regarding transport limitations and mechanical degradation due to intercalation-induced swelling. To enable next generation cell development, multidisciplinary design approaches are necessary, to couple and reconcile electrochemical and thermal performance with structural and geometrical constraints. This work presents a novel computational framework utilizing the open-source Python Battery Mathematical Modelling (PyBaMM) library to perform rapid Multi-Objective Optimization (MOO) of LIB cell geometry. The standard PyBaMM electrochemical solver which allows for the dynamic prediction of cell thickness change was extended using a set of composite descriptors, including current-non-uniformity indices, peak swelling strain and surface strain rate. A systematic parameter sweep focusing on electrode thickness as the primary design variable was implemented. By analysing distinct thickness configurations alongside a baseline design under 0.5C-2.0C, the Pareto frontiers quantifying the conflicting objectives of maximizing energy density and minimizing structural degradation and temperature gradients where established. The results uniquely quantify the non-linear relationship between electrode thickness and cell performance, giving critical insights into understanding the threshold where transport polarization and mechanical expansion outweigh the benefits of increased active material loading. This study contributes a robust methodology of multidisciplinary optimisation, demonstrating how coupled models can be effectively leveraged to determine optimal electrode geometries that satisfy both performance targets and mechanical constraints.

Keyword: Lithium-ion batteries, PyBaMM, Multi-Objective Optimization (MOO), electrode thickness, mechanical swelling

Probing inhomogeneous rocksalt growth using structure-resolved simulations

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Abstract

Ni-rich cathode materials are widely used in lithium-ion batteries due to their high energy and power density. However, the material stability severely limits their lifetime, especially when cycling to high cutoff voltages [1]. A layered-to-rocksalt transformation at the particle surface, accompanied by the loss of lattice oxygen, has been observed experimentally at low states of lithiation [1,2]. Recent experimental work revealed an inhomogeneous lithiation due to an inhomogeneity in rocksalt growth on single particles [3]. In real electrode structures, these particles are embedded in a complex electrode matrix with a concentration and potential distribution influenced by microstructural features such as particle size distribution, conductive additives or tortuosity. To investigate electrode degradation under realistic conditions, computational simulation tools can be availed.

In this contribution, we present a novel modeling approach to describe oxygen release and phase reconstruction in Ni-rich cathode materials [4]. The model was first implemented in a P2D approach and further extended to our simulation framework BEST [5] for 3D microstructure-resoled simulations. By applying our modeling approach to a high-resolution FIB-SEM tomography of a commercial Ni-rich cathode [6], we demonstrate how transport processes in realistic electrodes cause inhomogeneous phase reconstruction across the electrode. We will further discuss the impact of particle size and particle position on the predicted rocksalt growth as well as inhomogeneous degradation on the particle scale that results from inhomogeneous lithiation [7].

References:

[1] R. Jung et al., *J. Electrochem. Soc.*, 164 (7), A1361- A1377 (2017)
[2] S.-K. Jung et al., *Adv. Energy Mater.*, 4,1300787 (2014)
[3] Z. Lun et al., *Energy Environ. Sci.*, 18, 4097–4107 (2025)
[4] S. Both et al., *Batteries & Supercaps*, 8 (8), e202400802 (2025)
[5] A. Latz and J. Zausch, *J. Power Sources*, 196, 3296-3302 (2011)
[6] A. Lindner, S. Both et al., Batteries & *Supercaps*, 7 (12), e202400503 (2024)
[7] S. Both et al., *ChemRxiv*, https://doi.org/10.26434/chemrxiv-2025-jjm7q (2025)

Keywords: ModVal2026, Lithium-ion batteries, Ni-rich cathode materials, Rocksalt growth, Structure-resolved simulations

Battery Parameter eXchange (BPX):
a flexible standard for battery modelling and parameterisation

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The battery simulation landscape is fragmented, with many users running custom implementations of models. Battery Parameter eXchange (BPX) is an open, standardised framework that makes physics-based battery modelling compatible across different research and commercial simulators. At present, The Faraday Institution (UK) is supporting the development of BPX, with the intention that BPX will eventually become a standards body in its own right.

Based on a human-readable JSON schema, the first version of the BPX standard was released in July 2025, addressing the DFN, SPM and SPMe models. In addition, to preserve flexibility, BPX allows the use of user-defined parameters within the schema. Further work to expand the standard to cover experimental parameter determination and degradation models is under way.

Poster Abstracts

Session A: Energy Storage

Session A4: Next generation

Accelerating Lithium-Ion Battery Simulation with Neural Operators

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Abstract

As battery digital twins scale toward real-time predictive control and design, there is a critical need for surrogates that maintain physical fidelity at sub-millisecond computational speeds. We present a benchmarking study of machine learning surrogates for the Single Particle Model (SPM), introducing a novel Parameter-Embedded Fourier Neural Operator (PE-FNO). Unlike standard operators, the PE-FNO conditions spectral layers on physical properties—specifically particle radius and solid-phase diffusivity—to enable generalization across varying cell designs.

We evaluate performance against DeepONets, standard FNOs, and U-Net baselines across four diverse current profiles (constant, triangular, pulse-train, and Gaussian-random-field) over a 0–100% State-of-Charge range. Results demonstrate that while DeepONets struggle with highly dynamic loads, the PE-FNO maintains voltage Mean Absolute Errors (MAE) under **1.7 mV** and concentration errors below **1%**. Crucially, the PE-FNO achieves a **200x speedup** over a 16-thread numerical solver. To validate its utility in system-level applications, we demonstrate a parameter estimation task using Bayesian optimization, recovering electrode diffusivities with high precision. This work establishes PE-FNO as a high-performance alternative to classical solvers, meeting the accuracy, speed, and parametric flexibility demands of next-generation battery management systems.

Keywords: Physics-informed machine learning, Operator learning, Deep Operator Network, Fourier Neural Operator, Lithium-ion batteries

Pre-emptive Data Infrastructure Enables Model Validation at Scale: Insights from a Battery Startup

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Abstract

Validation of battery models requires diverse data spanning multiple chemistries, formats, and conditions. Across four years, Echion has accumulated data from approximately 19,000 cells, 4,000 material syntheses, and 60,000 characterisation files. However, this wealth of data becomes inaccessible without systematic data management infrastructure.

While tools exist to address specific aspects - materials databases for composition tracking [1]; code for standardising electrochemical data formats [2]; open-source physics-based cell models [3]; ML algorithms for lifetime predictions [4] - these tools often operate in isolation. Without connecting systems, researchers face compounding problems: proprietary file formats fragment datasets; missing metadata prevents searching for specific test conditions; and inconsistent analysis methods compromise reproducibility.

This work demonstrates a proactive approach to data management through three stages:

- **Automated standardisation**: We developed >10 processing pipelines covering electrochemical (life cycling, rate tests) and physicochemical (XRD, SEM, BET) characterisation, automatically parsing proprietary formats into standardised schemas.
- **Metadata capture**: Using familiar Excel interfaces, researchers tag experiments with synthesis details, compositions, electrolyte variations, cell formats, and protocols; this metadata is consolidated into a relational database searchable by validation-relevant parameters.
- **Accessible querying**: We deploy Metabase, an open-source platform, allowing modelers to query using natural language (e.g., "show all cells with Nb_2O_5 loading 3-4 mg/cm² cycled at 5C"). This system uses open-source tools deployable on a single server, making it accessible to academic groups.

By investing in pre-emptive standardisation and metadata capture, this workflow enables validation using historical datasets that would otherwise require weeks of manual compilation or costly re-testing.

[1] Jain et. al. (2013), *APL Materials, 1(1)*, DOI:10.1063/1.4812323
[2] Holland, T. et. al. (2025), *Journal of Open Source Software*, 10(106), DOI:10.21105/joss.07474
[3] Sulzer et al. (2021), *Journal of Open Research Software*, 9(1), 14. DOI:10.5334/jors.309
[4] Herring et al. (2020), *SoftwareX*, 11, 100506. DOI:10.1016/j.softx.2020.100506

Keywords: ModVal2026, Data infrastructure, Metadata standardisation, Open-source tools

Electrochemical performance modelling of fast-charging niobium-powered applications using PyBaMM

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Abstract

Niobium-based batteries offer a promising solution for heavy-duty electrification (e.g. mining vehicles and trains) due to their ability to withstand high-rate (>5C) charging without lithium plating, long cycle life, and intrinsic safety. Accurate prediction of their performance, degradation, and Total Cost of Ownership (TCO) requires physics-based models that can operate under fast-charging conditions.

Standard electrochemical models, such as the Single Particle Model with electrolyte (SPMe), often fail to capture the complex kinetics of niobium materials at high C-rates [1][2]. Furthermore, open-source tools like PyBaMM currently lack specific parameterisations for these novel chemistries [3]. This work closes the modelling loop from novel active material chemistries, through large-format cells, battery packs to predict performance in final application.

To achieve this, we extend the SPMe for a niobium-based anode and NMC cathode, implemented within the PyBaMM framework to simulate a large-format pouch cell at >5C performance, ultra-long cycle life, and a new chemistry. Key physics modifications include implementation of a concentration and rate-dependent diffusion coefficient to capture high-rate transport limitations [1] and application of a non-dilute (high concentration) approximation of the exchange current density [4] to the Butler-Volmer equation to account for electric double-layer effects.

Predicted values for capacity and DCIR at 10,000 cycles showed a maximum deviation of 3% from experimental benchmarks, and experimental validation from a road-tested niobium powered Toyota Landcruiser demonstrates voltage predictions within 38 mV RMSE across a 20-minute window. These results demonstrate the accuracy of our model applied to one of the first-real world applications of niobium-based batteries. Work is now underway to convert the model to a web-based applications to drive industrial engagement for this novel battery material.

Keywords: Niobium, fast-charging, modelling, PyBaMM

References:

[1] Maurits E. Houck, et.al. Parameterization and modeling protocols for ultra-fast charging Wadsley-Roth lithium-ion batteries from coin to pouch cells. Cell Reports Physical Science, 4, 5 2023.
[2] Maurits E. Houck. The thermodynamics, kinetics and modelling of fast-charging lithium-ion batteries featuring crystallographic shear niobium metal oxide anodes. PhD thesis, Apollo - University of Cambridge Repository, 2023.
[3] Valentin Sulzer et.al.. Python battery mathematical modelling (pybamm). ECSarXiv, February 2020.
[4] M. Z. Bazant, Accounts of Chemical Research, vol. 46, no. 5, pp. 1144–1160, 2013.

Theory-based Analysis of 1,4-Polyanthraquinone as Cathode Material for Post-Lithium Batteries

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Abstract

There is a variety of possible organic cathode materials for post-lithium batteries. One promising candidate is 1,4-polyanthraquinone (PAQ), as suggested for example by Z. Zhao-Karger et al. [1]. Our research focuses on theory-based analysis of the material, by using density functional theory (DFT) methods to gain insights into its structure, and improve our understanding of its bonding properties with different metal ions used as anode materials.

For periodic DFT calculations, we considered different numbers of anthraquinone units in the unit cell of the polymer and searched for energetically comparable conformers. To achieve this, we developed a computationally efficient approach to generate these conformers for various numbers of anthraquinones in the unit cell, ensuring that no duplicates were created through symmetry or rotation. We then inserted different metal ions into these conformers and compared their energies and structures to unveil different performance capabilities of various post-lithium ions based on the atomistic behavior.

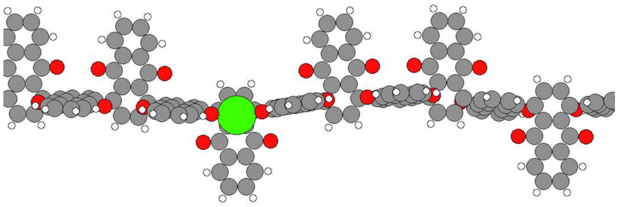

Figure: One PAQ conformer with one Calcium atom [Generated with 2, 3]

[1] Z. Zhao-Karger et al., Nat Commun 13 (2022), 3849.
[2] A. Larsen et al., J. Phys.: Condens. Matter 29 (2017), 273002.
[3] AMS 2024.101, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, Netherlands, www.scm.com.

Keywords: Organic Cathodes, DFT, Post-Lithium Batteries

PyBaMM-Based One-Dimensional Model for Morphological Evolution and Capacity Degradation in Li–S Cells

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Abstract

Lithium–Sulfur battery (LSB) is a superior alternative to Li-ion batteries due to its high specific theoretical capacity (1675 mAh/g) and specific energy density (2600 Wh/kg). However, the major roadblocks to the commercialization of Li–S batteries include poor capacity retention due to the polysulfide shuttle and rapid volume changes of the electrodes. In this work, we develop a one-dimensional Li-S cell to model to correlate the volume change in electrodes resulting from various electrochemical and chemical processes using PyBaMM. The model is parameterized and validated using the experimental dataset of Sylwia et al.[1]. Figure 1 shows the variation in cell voltage and thickness during the charge/discharge cycle. The linear compression of the cell during the high plateau discharge originates from the constant current stripping of the Li metal anode. A bump in the thickness profile is observed during the low plateau discharge, caused by the precipitation of Li_2S in the composite sulfur cathode. During charge, the cell expansion is mainly due to the non-uniform reduction of Li^+ ions at the Li-metal anode. The model captures capacity degradation during constant current cycling into three stages. In Stage I, the loss in discharge capacity is primarily due to the reversible polysulfide shuttle, which is completely recovered during the cell charge. Stage II includes capacity fade due to the irreversible loss of S_8^{2-} and S_4^{2-} species. The loss of such species hampers the charge capacity. Stage III involves drastic decay in charge capacity due to the high volumetric change in the anode, resulting in SEI formation and loss of active Li metal. These model observations can play a significant role in mitigating capacity fade by optimizing material selection and designing an effective charge protocol.

Keywords: ModVal2026, Lithium-Sulfur batteries, Shuttte effect, Dendrite growth

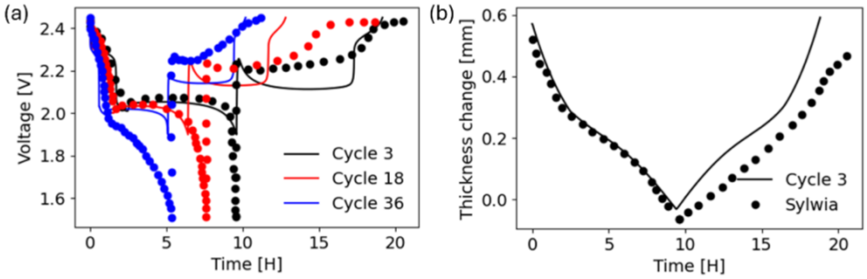

Figure 1: (a) Voltage curve and (b) the thickness change of 11 Ah OXIS Energy single-layer pouch cell.[1]

1. Waluś, S., Offer, G., Hunt, I., Patel, Y., Stockley, T., Williams, J., & Purkayastha, R. (2018). Energy Storage Materials, 10, 233–245.

Poster Abstracts

Session A: Energy Storage

Session A5: Particle cracking

Geometry dependence of effective transport in a periodic medium

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Abstract

In order to investigate the influences of cracked particles on the electrode scale we first focus on a single particle. The cracks within said particle can be categorized as intergranular cracks, i.e. cracks along grain boundaries which are often in a star-shaped pattern, or as intragranular cracks, cracks within a grain and generally aligned with a crystallographic plane.

To investigate the influence of intragranular cracks in active material particles on the transport within, a known homogenisation method for porous media [1] was utilized for two and three dimensional rectangular and cuboidal domains. The cracks were approximated by ellipses and spheroids, respectively. Calculating the effective material properties requires solving a specific set of differential equations on a periodic unit cell called a cell problem that is solved using a finite element based software. It was possible to construct a predictive analytical function based on the key geometrical crack properties: volume ratio, aspect ratio and angle of rotation and in the three-dimensional case the type of spheroid. The main obstruction to the transport is hereby given by the area the crack is shading in transport direction. This quantity is calculated utilizing orthogonal projections and is therefore called projected height or projected area, respectively. To include different types of active material the investigations were conducted for isotropic as well as different anisotropic material properties.

The investigation into intergranular cracked material was started focusing on simplified crack patterns like zigzag patterns of ellipses and ellipsoids. The transport properties of such cracked material follows a similar trajectory as the singular cracks. This is an encouraging result when it comes to the wider application of the aforementioned analytical predictive functions.

References:

[1] U. Hornung, Models for Flow and Transport through Porous Media Derived by Homogenization, Environmental Studies, Springer New York, 1996, pp. 201–221

Keywords: ModVal2026, effective transport, homogenization, cracked material, perforated domain

Accelerated Aging of LFP Batteries: Investigating Cathode Degradation Mechanisms

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Abstract

Lithium Iron Phosphate (LFP) batteries are gaining widespread adoption due to their thermal stability, safety, long cycle life and cost-effectiveness. While LFP chemistry avoids many degradation issues observed in high-nickel cathodes, aging phenomena still occur on the cathode side under demanding operating conditions. Despite its olivine structure providing good structural stability, LFP is susceptible to particle cracking, localized phase transformations and iron dissolution, particularly during high C-rate operation and extended cycling at elevated temperatures. These degradation mechanisms lead to capacity fade, impedance growth and loss of active material, making the understanding of LFP degradation important for optimizing energy storage and electric mobility applications.

In this study, controlled cycling tests under operating conditions known to cause accelerated cathode degradation were used on LFP‖graphite cells. Aging protocols were designed using a framework where one parameter was varied at a time (such as temperature, charge and discharge rates, and state-of-charge cycling window), to capture the effects of real-world operating conditions. Non-invasive electrochemical diagnostic techniques, including EIS, differential capacity analysis and differential voltage analysis, were used to monitor performance evolution during aging, while post-mortem SEM/EDS, XRD and XPS analyses identified morphological and chemical degradation signatures.

Although the study is primarily focused on cathode degradation, the anode was also examined. Degradation phenomena such as lithium plating and structural degradation were observed on the anode side under high-stress operating conditions, making complete decoupling of electrode-specific aging challenging in full cells, especially when using non-invasive techniques. The combined electrochemical and materials characterization enables correlation between the applied stressors and degradation mechanisms, providing insights into mitigation strategies to improve LFP cathode stability and overall cell durability.

Keywords: Lithium Iron Phosphate (LFP) batteries, cathode degradation, accelerated ageing, post-mortem analysis

Beyond Paris's Law: rethinking particle cracking, active material isolation, and degradation in lithium-ion cells by a mechanically coupled LAM model

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Abstract

Predicting the life of lithium-ion cells is a critical challenge in electrochemical modelling due to the complex interplay of multiple electrochemical and mechanical processes. Loss-of-active-material (LAM) due to particle cracking and electrical isolation is one of the critical degradation modes responsible for capacity loss and must be incorporated into a well-coupled degradation model. Many existing LAM models are weakly coupled within the Doyle–Fuller–Newman (DFN) framework, require heavy parameterisation, suffer from numerical instability, and assume Paris' law behaviour for cracking, which recent studies [1] indicate may not hold.

To address this, we present a unified, mechanically coupled LAM model, developed and fully integrated into the DFN framework using PyBaMM. Inspired by previous studies [2,3], our model couples cracking and isolation directly to particle stress and specific surface area (SSA) evolution. The model also dynamically updates average electrode particle radii, solid-phase diffusivities, and the ionic and electronic conductivities of the electrodes to better couple it to the DFN framework and make it more fundamentally grounded than previous LAM models in PyBaMM.

The model reproduces behaviour predicted by experimental and modelling results from Karger et al. [1] and shows that cracking leads to an initial rise in SSA, which eventually decreases as isolation dominates. Consistent with Karger et al. [1], the model predicts that the particle cracking rate decreases with cell cycling and does not follow the popular Paris' law. This work provides a new framework to study particle- and electrode-level mechanical degradation and is particularly relevant for large-particle-radius chemistries and fast-charging applications. The model is numerically stable, physically interpretable, and easier to parameterise than existing LAM models in PyBaMM.

Keywords: *ModVal2026, loss of active material (LAM), particle cracking and isolation, mechanical degradation, PyBaMM, specific surface area, fast charging, Paris's law, DFN*

References:

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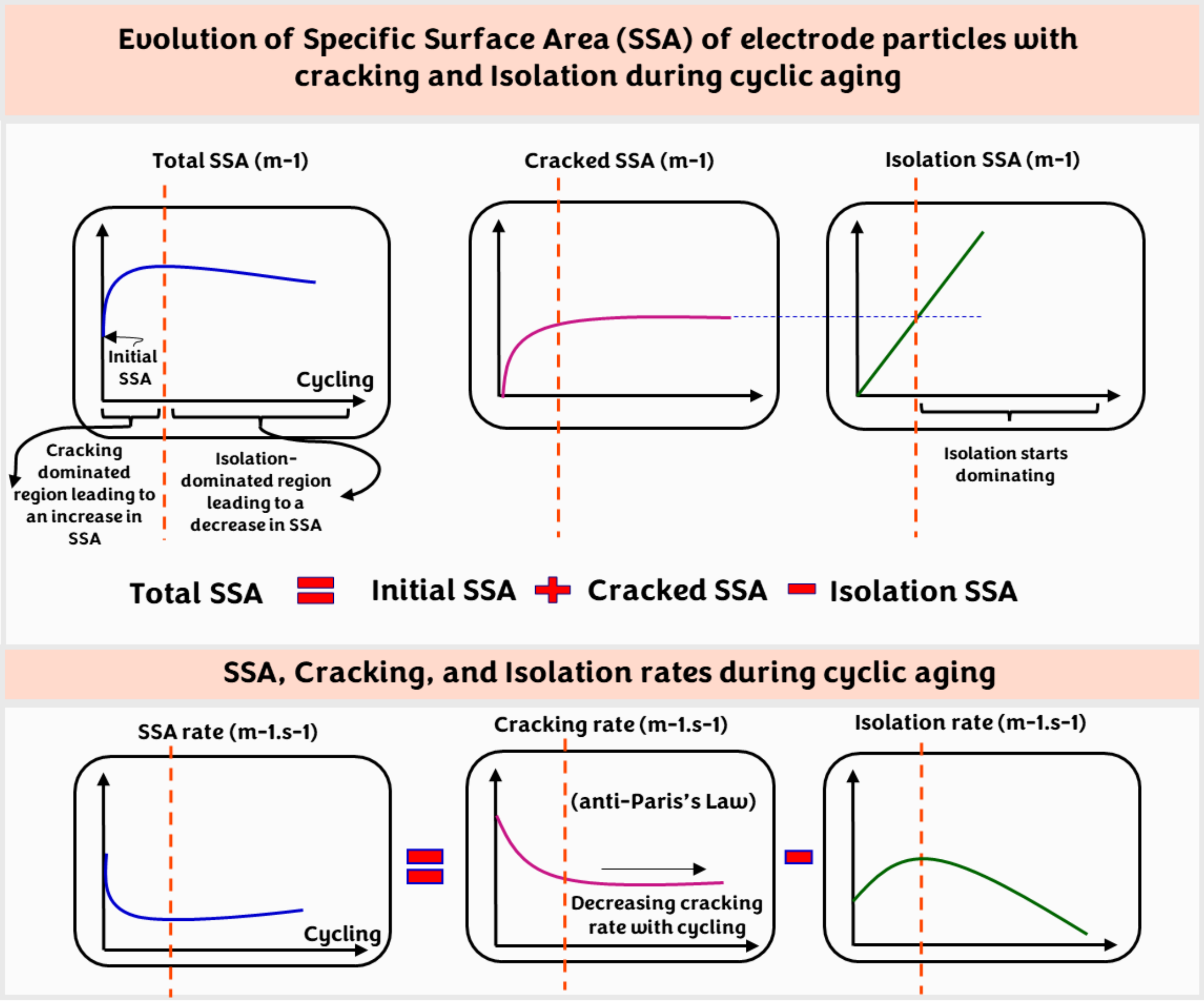
[1] Karger, A. et al. Modeling particle versus SEI cracking in lithium-ion battery degradation: why calendar and cycle aging cannot simply be added. J. Electrochem. Soc. 171, 090512 (2024). https://doi.org/10.1149/1945-7111/ad76da

[2] Barai, P., Smith, K., Chen, C.-F., Kim, G.-H. & Mukherjee, P.P. Reduced order modeling of mechanical degradation induced performance decay in lithium-ion battery porous electrodes. J. Electrochem. Soc. 162, A1751–A1762 (2015). https://doi.org/10.1149/2.0241509jes

[3] Narayanrao, R., Joglekar, M.M., & Inguva, S. A phenomenological degradation model for cyclic aging of lithium ion cell materials. J. Electrochem. Soc. 160, A125–A137 (2013).

Supplementary Info



Visualisation plot created using simulation done using the developed LAM model in our current work in PyBaMM: Plots demonstrate that cracking increases the total SSA, and isolation decreases it; the competition between the two governs the net change in SSA. The particle cracking rate decreases with cell cycling, demonstrating cracking behavior of the electrode does not follow the popular Paris' law.

Poster Abstracts

Session A: Energy Storage

Session A6: Thermal impact

Temperature dependence of tortuosity measurements for different electrode types under compression

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Abstract

The tortuosity of porous electrodes of lithium-ion batteries is typically determined using an impedance-based symmetric cell method proposed by Landesfeind et al. [1] in 2016. This method is considered superior over imaging-based approaches due to its sensitivity for the carbon binder domain. To satisfy the requirement of negligible electronic resistance in the solid phase, electrolytes whose ionic conductivities lie one order of magnitude below the range of their commercial counterparts are used.

Hitherto, literature has suggested that tortuosity determination via this method is largely independent of the conductivity of the electrolyte used [1,2]. Therefore, tortuosity determination in recent research work was conducted at various temperatures and with electrolytes of different conductivities.

Using a symmetric, single-layer setup with commercial NMC, graphite, and LFP electrodes that enables highly reproducible results, we uncovered a possible dependence of tortuosity results on electrolyte conductivity and temperature. This dependence was only observed for NMC and graphite electrodes, and not for LFP electrodes. The reason why this dependence is only observed for certain electrodes is still unclear. However, this behavior could represent an additional mechanism influencing temperature-dependent performance of lithium-ion batteries. To accurately assign polarization to physicochemical processes and obtain reliable parameters for modelling, it is therefore necessary to better understand this anomaly.

Our work suggests that tortuosity determination of pristine electrodes should be conducted with the electrolyte, used in the cell, to be parameterized. This is, however, only possible if electronic conductivities of the electrodes are sufficiently high, to be neglected. We hope that our results can initiate an in-depth investigation of the mechanisms causing this behavior for certain electrodes.

Keywords: ModVal2026, tortuosity, lithium-ion battery, microstructure

[1] Landesfeind, Johannes, et al. "Tortuosity determination of battery electrodes and separators by impedance spectroscopy." *Journal of The Electrochemical Society* 163.7 (2016): A1373.

[2] Landesfeind, Johannes, et al. "Tortuosity of battery electrodes: validation of impedance-derived values and critical comparison with 3D tomography." *Journal of The Electrochemical Society* 165.3 (2018): A469-A476.

High-Fidelity Modeling of Cell-Level Thermal Runaway in Lithium-Ion Batteries

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Abstract

The rapid expansion of battery applications in transport and stationary storage has renewed attention on safety, particularly the mechanisms leading to thermal runaway (TR). Recent reviews on battery thermal management [1] and cell failure behaviour [2] highlight that TR is driven by strongly exothermic reactions and the release of flammable gases, which can lead to ignition, pressure rise and structural damage. Although many modelling approaches examine TR at the module or system level, the need for robust tools capable of predicting and mitigating TR events at the cell level has become more pressing [1, 2, 3]. This work develops a numerical framework to investigate TR at the cell level using Large Eddy Simulations (LES) implemented in OpenFOAM. The configuration follows the experimental setup and reduced-order modelling strategy proposed by Cellier (2023) [3] and allows a coupled simulation of heat release, gas venting and internal flame development. The model accounts for reactive gas dynamics, pressure evolution and anisotropic heat transfer. It also includes the influence of geometric confinement on flame behaviour, consistent with the analyses reported in recent studies [4, 5]. Thermochemical inputs and boundary conditions rely on the experimental data provided in [2], particularly concerning the influence of cathode composition on gas release and ignition thresholds. Additionally, key design features, such as the vent opening and the thermal response of the casing, were varied to examine how they influence the gas release and the redistribution of heat during a TR event. These analyses help clarify the conditions under which internal failure develops and point to design adjustments that can enhance protective structures and the positioning of diagnostic sensors. By resolving cell-level processes with higher physical fidelity, the result from this study reduces uncertainties in existing predictions and contributes to assessment tools for emerging battery technologies with an increased reliability.

Keywords: Thermal runaway, OpenFOAM, LES, flame propagation, lithium-ion batteries, cell-level simulation, validation

Acknowledments:
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References:

1. Li, W., Zhou, Y., Zhang, H. and Tang, X., (2023). A review on battery thermal management for new energy vehicles. Energies, 16(13), p.4845.

2. Golubkov, A.W., Scheikl, S., Planteu, R., Voitic, G., Wiltsche, H., Stangl, C., Fauler, G., Thaler, A. and Hacker, V., 2015. Thermal runaway of commercial 18650 Li-ion batteries with LFP and NCA cathodes–impact of state of charge and overcharge. Rsc Advances, 5(70), pp.57171-57186.
3. Cellier, A., 2023. Simulation aux Grandes Echelles de Feux de Batteries Lithium-ion pour le Diagnostic de l'Emballement Thermique (Doctoral dissertation, Institut National Polytechnique de Toulouse-INPT).
4. Illacanchi, F., Valencia, S., Celis, C., Mendiburu, A., Bravo, L. and Khare, P., 2023. Numerical Study of Distorted Tulip Flame Propagation in Confined Systems. arXiv preprint arXiv:2309.05893.
5. Liberman, M.A., Qian, C. and Wang, C., 2022. On the formation of a tulip flame in closed and semi-open tubes. arXiv preprint arXiv:2209.00709.

PCM-Based Thermal Energy Storage for Thermal Management of Heavy-Duty Batteries

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Abstract

Thermal management is critical for ensuring performance, safety, and durability in heavy-duty vehicles (HDVs) battery systems, which experience high thermal loads during operation. This study experimentally investigates a phase change material (PCM)-based thermal energy storage (TES) system as a passive solution for battery thermal management (BTM). Five commercial PCMs were thermally characterized through differential scanning calorimetry (DSC), thermal conductivity measurements, and cycling stability tests.
N-octadecane emerged as the most suitable candidate, exhibiting a melting range of 25–32 °C, high latent heat (≈222 J g^{-1}), and excellent thermal durability over 20 cycles. A dedicated fin-and-tube TES system filled with n-octadecane was tested under various heat-transfer-fluid (HTF) flow rates (2–3 L min^{-1}). Results showed that heat transfer was conduction-dominated in the solid state and strongly convection-enhanced in the liquid state. While HTF flow rate had limited impact on total charging/discharging times, it significantly improved thermal power output. At 3 L min^{-1}, the TES achieved a thermal power ratio of 56, alongside substantial performance gains compared to the no-PCM baseline: a 3.5× increase in gravimetric specific power (0.056 kW kg^{-1}) and a 6× increase in volumetric specific power (approximately 68 kW m^{-3}). Overall, the findings validate n-octadecane as a promising PCM for passive thermal buffering in HDV battery systems and highlight the potential of modular PCM-TES units as scalable solutions for battery pack cooling or cabin thermal management.

Keywords: ModVal2026, phase change material, battery thermal management, thermal characterization, thermal energy storage.

Reduced-Order Thermal Modeling of Cylindrical Lithium-Ion Battery Cells: An Experimentally Economical Approach

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Abstract

Despite their technological maturity, accurate prediction of the electrical and thermal behavior of lithium-ion batteries remains challenging, particularly under the highly dynamic operating conditions encountered in personal motor vehicles. High and irregular currents during acceleration, regenerative braking, and fast charging can lead to significant internal heat generation, making effective thermal management essential. Cell temperature directly impacts performance, lifetime, and safety, with excessive internal temperatures potentially leading to severe degradation or, in extreme cases, thermal runaway. While surface temperature can be measured directly, internal temperature typically must be inferred through modeling or indirect measurement techniques.

In this work, a reduced-order thermal modeling approach is developed to quantify both heat generation and internal heat propagation in cylindrical lithium-ion battery cells. The proposed model adopts an experimentally economical approach, relying primarily on standard cell characterization data commonly obtained during routine testing, including open-circuit voltage, capacity, and pulse power measurements. The framework is augmented by one additional laboratory experiment to determine the entropic coefficient of the cell and an experiment to identify the thermal boundary condition parameters, supplemented with parameters drawn from literature.

Heat generation is modeled by accounting for both irreversible losses due to overpotential, represented via an equivalent circuit model, and reversible entropic heating. Heat propagation and dissipation within the cell are captured using a two-dimensional finite-element lumped thermal model. The complete modeling pipeline is implemented in Python and supports laboratory data ingestion, synthetic load profile generation, computationally efficient data handling, and result visualization.

Validation was conducted under ambient conditions using a dynamic test profile representative of vehicle operation. The profile comprises a 1.5C fast charge from 10 to 80% state of charge, followed by a relaxation period, a two-stage drive-cycle discharge back to 10% state of charge, and a final relaxation phase. Model predictions were evaluated at three locations on the cell against corresponding thermocouple measurements, yielding an overall root-mean-square error of 1.4 K and a mean absolute error of 1.2 K.

Keywords: ModVal2026, lithium-Ion batteries, thermal modeling, internal temperature estimation, battery thermal management, electric vehicles

Influence of Thermal Gradient Direction during Aging on the Thermal Conductivity of Blend-Cathodes

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Abstract

For an efficient and safe operation of lithium-ion battery systems in electric vehicles a thermal management system is required. The design of thermal management systems is thereby commonly based on the respective cell behavior and properties at the Begin of Life (BoL) ignoring possible changes of the thermophysical properties during aging. These might even be enhanced by the thermal management system, which inevitably imposes thermal gradients within the battery cells.

The direction of thermal gradients in relation to the electrode layers of the cell stack or jelly roll can have a significant influence on the aging. Compared to the in-plane gradients, the through-plane gradients show more severe aging mechanisms. To assign the occurring aging mechanisms to the changes of the thermophysical properties, it is crucial to measure the electrodes individually because of the different aging mechanisms within anode and cathode. Using an in-house developed experimental methodology for the thermal characterization at electrode level the effective thermal conductivity can be determined by measuring the specific heat capacity with differential scanning calorimetry, the density with a gas pycnometer and the thermal diffusivity with laser flash analysis.

In order to investigate the influence of thermal gradients and the gradient direction on the changes of the thermophysical properties of lithium-ion battery electrodes, this study systematically analyzes cyclic aged cells under various inhomogeneous thermal conditions and compares them with the properties at BoL. The investigated commercial pouch cells (20 Ah) consist of graphite anodes and blend metal oxide cathodes. Additionally, the impact of homogeneous thermal conditions during aging is investigated to identify the specific contribution of thermal gradients to the aging induced changes of the nickel-manganese-cobalt (NMC) and lithium-manganese oxide (LMO) blend-cathode. Several samples were taken from the differently aged cells at the End of Life and the corresponding effective thermophysical properties are determined using the described methodology. With an according post-mortem analysis, the changes of the effective thermal conductivity are assigned to the occurring aging mechanisms on electrode level.

Keywords: Lithium-Ion Batteries, Aging, Thermal Gradients, Thermal Conductivity

Thermal Conductivity Evolution of Lithium-Ion Pouch Cells over Lifetime

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Abstract

Through-plane thermal conductivity of a lithium-ion battery changes significantly throughout its life, but the magnitude of change is highly dependent on the ageing conditions and loads applied to the cell. Accurately accounting for the evolution of thermal properties is essential for predicting cell temperature rise under different operating conditions. Neglecting changes in thermal properties during ageing can lead to large errors in degradation models, particularly because battery degradation mechanisms are highly temperature dependent. In this study, ten large format lithium-ion pouch cells are aged under controlled conditions, including different temperatures and electrical loads, while maintained under compression. Periodic measurements of through-plane thermal conductivity are performed alongside electrical characterisation throughout ageing. Thermal conductivity evolution is correlated with degradation modes extracted from pOCV analysis, including loss of lithium inventory (LLI) and loss of active material in both electrodes (LAM_{PE}, LAM_{NE}). By linking thermal property changes to specific degradation mechanisms, this research enables improved prediction of thermal behaviour over a battery's life, supporting more accurate degradation modelling and optimised battery pack and thermal management design.

Keywords: Lithium-ion Battery, Degradation, Ageing, Thermal Conductivity

Instructions:

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4. **Add your specific keywords** at the end of the document, after the given keywords:
   Keywords: ModVal2026, proton exchange membrane electrolyser, solid oxide fuel cell, …

Identifying and Developing Standards for Electrochemical and Empirical Battery Model Validation

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Abstract

This work identifies incomplete specification of thermal boundary conditions as a structural weakness in current battery model validation practice. Validation commonly treats the heat sink or ambient temperature as the presumed cell temperature, thereby introducing a thermal error that is inseparable from electrochemical parameter error in reported validation metrics. Unlike parameter error, which is intrinsic to model structure and identifiability, thermal error is induced by the validation procedure itself and undermines reproducibility and comparability across laboratories, thermal control strategies, and model classes. We argue that explicit thermal environment characterisation is a missing prerequisite for credible and standardisable model validation of electrochemical cells.

We propose a validation protocol in which the thermal environment is parameterised prior to electrochemical model assessment. A dedicated pre-validation experiment is introduced to characterise the effective heat transfer pathway between the cell and its thermal management system. Controlled current pulse protocols are used to generate repeatable heat generation and achieve elevated thermal steady-state conditions, from which an effective heat transfer coefficient is identified. This coefficient defines a lumped thermal boundary condition that can be coupled with an otherwise standard electrochemical or empirical model via a thermal resistance, isolating thermal boundary uncertainty without increasing battery model complexity.

The approach is demonstrated across multiple thermal management configurations, including insulated and surface-cooled environments. Initial numerical work has highlighted that the inclusion of a characterised thermal boundary improves correlation between predicted and measured cell performance during validation experiments. We hypothesise that the magnitude of improvement depends on the thermal control strategy used in validation, with the largest reductions observed where thermal control is least powerful (e.g. benchtop or climate chamber). Residual discrepancies are consistent with unresolved differences between surface and effective internal cell temperature, indicating that both internal and external gradients must ultimately be addressed to fully eliminate thermal error from a model performance. These results support thermal environment characterisation as for inclusion in emerging battery model validation standards.

Keywords: Thermal control, thermal models, validation experiments

Poster Abstracts

Session B: Energy Conversion

Session B1: High-temperature electrolysis

PressHyous – Pressurized hydrogen produced by high temperature steam electrolysis

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Abstract

The production and use of clean H2 is a key lever for the decarbonation of industries, as a fuel for transportation and as a storage vector for renewable electricity at large scale. The RePowerEU plan, for saving energy, producing clean energy, and diversifying energy supplies sets out a strategy to double the previous EU renewable H2 target (10 million tons/y of domestic production +10 million tons/y of H2 imports). Meeting these targets requires the EU to significantly upscale its manufacturing capacities for innovative equipment such as electrolysers.

However, using H2 requires given levels of pressure depending on applications. Thus to pave the way to the delivery of down to zero emissions of pressurised H2 at reduced cost (around 3 €/kg by 2030), PressHyous will validate the operation of a 20 kWe pressurised lab-scale device (eq. 13.5 kg H2/d) composing of a solid oxide electrolyser (SOEL) stack placed in a pressurised vessel, up to 30 bar at 1 A/cm2 and 1.3V during 4000h. PressHyous will also investigate a promising pressurised stack concept (without pressure vessel) relieving the cost of Balance of Plant. This will be tested up to 10 bar at short stack scale, at a similar current density to the stack operated in a pressurised vessel. These two stacks will integrate optimised components such as cell and sealing. PressHyous will in parallel deliver model-based insights for H2 production under pressure for up to 5 identified use cases, on expectable performances of both stack concepts (with or without pressurised vessel) towards large scale developments up to 100s MWe, in strong link with techno-economic and life-cycle analysis.

PressHyous consortium gathers a large portfolio of skills from modelling to system manufacturing, and a wide range of partners (RTOs and industrials) all along the value chain. The scientific and technological activities are all intended to strive towards the overall design and validation of future MWe large scale pressurised SOEL.

Keywords: ModVal2026, pressurized conditions, solid oxide electrolysis, hydrogen production

Parameter Identification and Modeling of Solid Oxide Electrolysis Segmented Cells

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Abstract

Non-uniform distributions of current and temperature within solid oxide electrolysis cells (SOECs) are major factors accelerating electrode degradation and causing thermo-mechanical failure. A thorough analysis of the local characteristics of the multi-physics is therefore essential for improving cell performance and extending operational lifetime. In this study, a three-dimensional numerical model is developed based on an anode segmented-cell test platform, enabling elucidation of the coupling between local electrochemical behavior and the current in the segmented cell. Utilizing extensive impedance spectroscopy data obtained from six-segmented cells, key electrochemical parameters—including the partial-pressure dependence exponents of the cathode and anode exchange current densities and temperature-dependent pre-factors—are identified by fitting a semi-empirical power-law model. Comparison with in-situ segmented-cell test results demonstrates that the model accurately predicts I-V characteristics and EIS responses across a wide range of operating conditions. The results indicate that the model reliably captures activation polarization over broad temperature and gas-composition ranges. Consequently, high-precision identification of local electrochemical parameters provides a robust foundation for judgment of adverse working conditions and the evaluation of the optimization design and operation strategy of SOEC.

Keywords: SOEC modelling, segmented cells, parameter identification

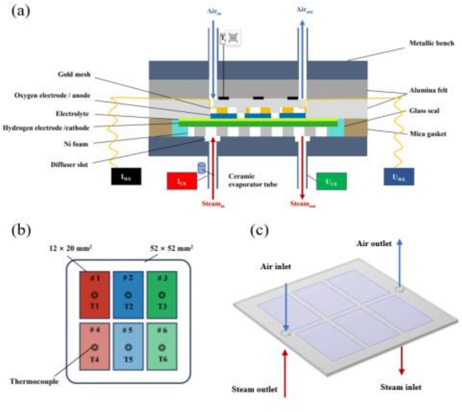

Figure 1: (a) Experimental setup used for the SOEC operation. b) 3D SOEC model schematic diagram. and (c) schematic of the 27.04 cur anodesupported cell with 6 cathode segments and 6 thermocouples at the center of each segment.

Solar-Driven Hydrogen Production Using a Molten Carbonate Electrolyser

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Abstract

Molten carbonate cells show significant potential for hydrogen production. Their strong performance at low current densities makes them particularly well suited for operation in endothermic mode. This characteristic can be exploited in combination with a solar cavity, creating a system that harnesses solar energy for hydrogen generation. In this work, the development of such a system is investigated. A zero-dimensional (0D) model of a molten carbonate electrolyzer was first developed. Particular attention was put on the electrochemical modelling: instead of the traditional voltage balance approach, a reduced-order model was adopted due to its improved capability to accurately predict open-circuit voltage (OCV) values. Combined with mass and energy balances, the model was compared against experimental data at different operating temperatures. The model showed very good agreement (R^2=0.97) with experimental results, except at 575°C, where an exponential behaviour was observed in the experimental data. In parallel, a solar cavity model was developed using the radiosity method, enabling the computation of different temperatures on the inner cavity surfaces. This model was also compared with experimental data and demonstrated high accuracy in predicting the thermal efficiency of the solar cavity across the entire temperature range, with a computed $R^2 = 0.99$. Finally, the integration of the two models was investigated, paving the way for a more in-depth analysis of the proposed system.

Keywords: Molten Carbonate Electrolyser; Solar-Driven Systems; Hydrogen Production

Poster Abstracts

Session B: Energy Conversion

Session B2: High temperature fuel cells

0D model for predicting sulphur-contaminant degradation in biogas-fuelled SOFCs

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Abstract

Hydrogen technologies and high-temperature Solid Oxide Fuel Cells (SOFCs) are key options for efficient, low carbon power, especially when operating on hydrogen and fuel-flexible feedstocks such as biogas. However, trace contaminants in biogas can poison the fuel electrode and accelerate performance decay, still limiting long-term operation. While some studies clarify poisoning mechanisms, compact predictive models able to reproduce the cell response and extrapolate beyond tested conditions remain scarce.

This work combines a targeted experimental campaign with a 0D degradation model. A single SOFC was operated on biogas doped with representative sulphur species, namely carbonyl sulphide (COS) and dimethyl sulphide (DMS), at two concentration levels (low and high) for calibration and validation. Performance decay is monitored via cell voltage-time curves. Electrochemical Impedance Spectroscopy (EIS) and current-voltage (IV) curves are acquired at the beginning and end of life. EIS data are processed in SOCEIS tool using Distribution of Relaxation Times (DRT) analysis combined with complex non-linear least squares (CNLS) fitting of an equivalent circuit. The analyses indicate that, under the investigated conditions, sulphur predominantly increases anode activation losses. Therefore, the model attributes the voltage drop to a change of the anode exchange current density.

Sulphur surface coverage is described through a Temkin-like isotherm linking coverage θ to temperature and to the partial-pressure ratio $\frac{p_{cont}}{p_{H_2}}$:

$$\theta = 1.45 - 9.53 \cdot 10^{-5} T + 4.17 \cdot 10^{-5} T \ln\left(\frac{p_{cont}}{p_{H_2}}\right)$$

A contaminant-specific correction factor modifies this relation to capture the different poisoning strengths of COS and DMS and improve agreement with experiments. Once identified from the two-level tests, the corrected formulation predicts cell behaviour at other contaminant concentrations, enabling practical performance forecasting for biogas-fueled SOFC systems.

Keywords: solid oxide fuel cells; sulphur poisoning; 0D degradation model

From Single Cell to System: Multiscale Analysis of Carbon Deposition in SOFCs

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Abstract

Solid Oxide Fuel Cells (SOFCs) offer a highly efficient and fuel-flexible route for sustainable power generation, making them particularly attractive for the utilization of carbonaceous fuels such as natural gas and biogas. However, long-term operation with carbon-containing fuels remains limited by degradation phenomena, including carbon deposition and metal dusting, which lead to performance losses and reduced durability. It is therefore crucial to understand how carbonaceous gases and the associated carbon deposition affect SOFC performance and degradation mechanisms from the single-cell level up to stack and system operation.

In this work, a multiscale experimental investigation is presented in which a single cell operated with internal methane reforming is compared with SOFC stack and system tests employing a partial methane reformer upstream of the anode inlet. A wide range of operating conditions, including temperature, gas composition, flow rate, and fuel utilization, has been explored, enabling identification of operating ranges that minimize carbon deposition. SOFC performance was evaluated by current-voltage characterization and electrochemical impedance spectroscopy (EIS). Long-term testing demonstrates performance degradation with different severities at the single-cell, stack, and system levels. Distribution of Relaxation Times (DRT) analysis and Complex Nonlinear Least Squares (CNLS) fitting were employed to deconvolute the individual electrochemical processes and identify those mostly influenced by carbon deposition, including ohmic resistance, gas conversion and gas diffusion resistance, and anode charge-transfer resistance. These analyses reveal that carbon deposition primarily affects triple-phase boundary (TPB) availability through blockage of active sites and may induce additional mass-transport limitations due to pore obstruction.

These results provide a consistent experimental basis for understanding and modeling carbon deposition effects across scales and support the development of mitigation strategies for SOFC systems operating on carbonaceous fuels.

Keywords: SOFC, Carbon deposition, EIS, Multiscale performance analysis

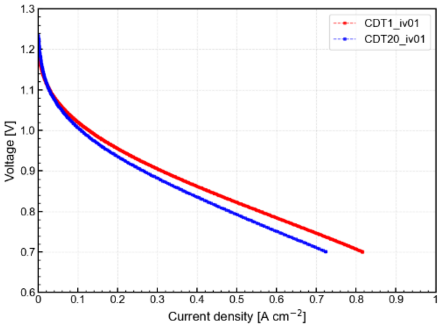

Figure 1 – SOFC single-cell degradation: IV curves before and after 20 biogas exposure cycles

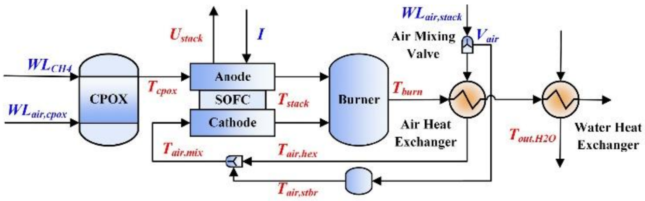

Figure 2 – Process flowsheet of the SOFC system under investigation

Modelling Approaches and Validation for Solid Oxide Cell Cross-Flow Stacks

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Abstract

Solid oxide cells (SOCs) are attracting increasing attention due to their high efficiency, fuel flexibility, and potential for integration into diverse industrial processes. Scaling from cell to system level is critical for industrial development, requiring deep understanding of system limitations, operating conditions that maximize performance and longevity. Laboratory cell and stack level experiments cannot fully capture these aspects. Likewise, lumped or simplified models derived from cell and stack models fail to account for spatial variations and interactions of key parameters and properties.

Among planar configurations, cross-flow stacks are particularly interesting because their design simplifies manifold integration and reduces passive area. However, they exhibit complex distributions of temperature, current density, and gas composition, which can only be captured through detailed 2D modelling.

Detailed modelling of SOCs at the reactor level is therefore essential to explore phenomena beyond the reach of experiments and lumped models and to develop effective operating and control strategies. The TEMPEST framework [1], developed by the German Aerospace Center in the object-oriented modelling language Modelica on the Dymola platform, addresses this need. The framework supports modelling from the cell to reactor level, with varying levels of detail and different planar configurations, such as co-flow and cross-flow, enabling thorough analysis of system dynamics, internal interactions and critical property distributions within cells and reactors.

This presentation demonstrates the application of the TEMPEST framework to a 2D + 1D cross-flow planar model for steady-state simulations and addresses the challenge of increasing model complexity when upscaling to the reactor level. The electrochemical properties of the investigated stack are validated through experiments conducted at different temperatures and pressures on a 10-layer cross-flow stack in the in-house pressurized test rig HORST [2]. A stack-level simplification approach previously presented in [3] is applied together with a novel cell level simplification that reduces the gas channels' discretization from 2D to 1D. These approaches reduce computational cost by more than 90% while maintaining less than 1% deviation in property distributions.

Keywords: Solid oxide cells (SOCs), Cross-flow stacks, Computational simplifications

1. F. Sedeqi *et al* 2024 *J. Electrochem. Soc.* **171** 074507
2. M. Riedel *et al* 2020 *J. Electrochem. Soc.* **167** 024504
3. M. Tomberg *et al* 2022 *J. Electrochem. Soc.* **169** 054530

Simulation of solid-state dewetting of thin nickel film in solid oxide fuel cells using phase field modeling

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Abstract

Nickel-yttria-stabilized zirconia (Ni-YSZ) is the most widely used fuel electrode material in solid oxide fuel cells (SOFCs) due to its excellent electrocatalytic activity. However, degradation of Ni-YSZ fuel electrode remains one of the major challenges hindering the large-scale commercialization of SOFCs. Dynamic Ni spreading and splitting with very high mobility under SOFC operation were observed in *operando* experiment of patterned Ni-YSZ cell, while Ni merely agglomerated by sintering under open circuit condition (Jiao & Shikazono, J. Power Sources 396, 119, 2018). Further investigations indicate the existence of an overpotential threshold, above which Ni migration is triggered under anodic polarization (Tao et al., Acta Materialia 305, 121867, 2026). Phase field modeling (PFM) is a useful approach for simulating microstructural evolution, and several models have been developed to simulate Ni-YSZ microstructure evolutions. In the present study, a phase field model incorporating Ni-YSZ interfacial wettability is developed to simulate solid-state dewetting of thin Ni film in patterned Ni-YSZ cell. Various perturbations are introduced to activate different instability phenomena during the dewetting process. The simulations demonstrate that distinct perturbations lead to different dewetting morphologies, governed by different instability mechanisms. These results provide more information of dynamic Ni morphological evolution observed under SOFC and are expected to contribute to a deeper mechanistic understanding of Ni migration degradation.

Keywords: solid oxide fuel cell, Ni-YSZ fuel electrode, solid-state dewetting, phase field modeling

In-situ simultaneous characterization of in-plane inhomogeneity of electrochemical performance and temperature field of solid oxide fuel cells

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Abstract

Solid oxide fuel cells (SOFCs) are a high-efficiency and clean energy conversion technology with significant commercialization potential. However, their long-term performance degradation and in-plane inhomogeneity limit practical deployment. Conventional testing methods cannot resolve the in-plane distribution of electrochemical performance and temperature, thereby making it difficult to accurately diagnose local degradation under operating conditions. To address this limitation, this study proposes and demonstrates an in-situ approach that combines segmented-cell testing with optical fiber temperature sensing to simultaneously characterize the in-plane electrochemical performance and temperature field of SOFCs. By varying the operating current, fuel flow rate and air flow rate, segment-resolved current-density and impedance responses are obtained, while embedded fiber Bragg grating (FBG) sensors enable real-time temperature measurement. As a result, the integration of segmented electrochemical characterization with optical fiber thermometry provides an effective method for revealing the dynamic evolution and underlying mechanisms of in-plane electrochemical–thermal inhomogeneity, thereby enhancing the visualization and early diagnosis capability of SOFCs under practical operating conditions.

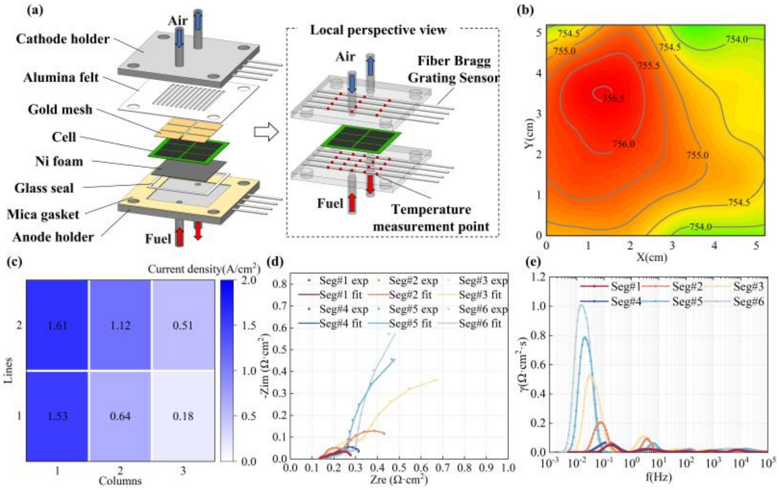

Figure 1: (a) Integrated setup of segmented-cell testing and optical fiber temperature sensor. (b) In-plane temperature distribution. (c) Local current-density distribution. (d) EIS of different segments. (e) DRT results of different segments.

Keywords: ModVal2026 (Solid oxide fuel cells, Segmented cell, Optical fiber sensor)

Modeling and validation of a packed bed reactor for catalytic oxy-combustion in a 10 kW SOFC+mGT system

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Abstract

Coupling a micro gas turbine (mGT) to the exhaust gases of a solid oxide fuel cell (SOFC) allows to retrieve even more electric power from the fuel feeding the SOFC. A patented design uses the anode off gases of the SOFC to produce a net work in a micro turbine followed by a compressor. The remaining fuel in the anode off gas, composed of approximately 11 mol% H2 and 2.5 mol% CO, is burnt using pure oxygen, thereby converting the chemical energy into thermal energy, which is then available to drive the expansion work in the mGT. Due to thermal constraints from the mGT, the burner exhaust gas temperature must be kept below 400°C. Considering the additional internal constraints, maintaining this outlet temperature is best achieved by a combination of burner cooling and steam injection. A novel catalytic burner design for oxy-combustion is developed and modelled using COMSOL Multiphysics.

This work focuses on modelling the catalytic combustion inside the burner and the influence of combustion conditions and dimensional parameters on the combustion performances. The challenge to model mass and energy transport in a packed bed reactor comes from the reactions occurring at the burner level and at the pellet level. For that, a 1D macroscale model is coupled to a 1D microscale model to address both mass and reaction distributions along the reactor and within the catalyst pellets.

The dimensional parameters of the burner and the pellets are found to allow for almost complete combustion. The working conditions, including variations of combustion regimes and reactor temperature confirm good combustion quality. Future work will focus on adding the cooling of the burner, improve thermal and chemical models, and perform dynamic modelling for the investigation of variations of working conditions. The simulation results will be validated with experimental data coming from an existing setup developed for the characterization of the burner alone.

Keywords: ModVal2026, catalytic combustion, oxy-combustion, SOFC exhaust combustion, packed bed reactor, SOFC+mGT system

A Dynamic 1D Modeling Framework for Reversible Solid Oxide Cells in OpenModelica

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Abstract

Solid Oxide Cell (SOC) technology is a key enabler for high-efficiency energy conversion and storage in advanced power-to-power (P2P) and power-to-X systems. The intrinsic advantages of SOCs - such as high operating efficiency, fuel flexibility, and reversible operation - are counterbalanced by significant challenges related to thermal management, system complexity, and balance-of-plant (BoP) integration. These challenges are particularly critical for reversible solid oxide cells (r-SOCs), which operate alternately in fuel cell (SOFC) and electrolysis (SOEC) modes and are therefore subject to strong thermal and electrochemical transients.

In this context, physics-based modeling is essential to support both system design and experimental validation activities. While steady-state 0D models are often used for preliminary system studies, their limited capability to capture spatially distributed phenomena and transient behavior restricts their applicability when investigating dynamic operation, thermal coupling, and off-design conditions.

This work presents the ongoing development of a dynamic, spatially resolved r-SOC model, conceived as an evolution of a previously validated steady-state 0D Matlab™ model. The new modeling framework is implemented in the Modelica language using the OpenModelica Editor (OMEdit) and introduces a 1D axial discretization of the cell, enabling a more detailed representation of thermal and electrochemical interactions between solid components and gas channels.

The model adopts a modular, object-oriented structure that facilitates progressive refinement and future extension toward stack-level simulations and experimental validation. Heat transfer mechanisms, including convective coupling between gas channels and solid layers as well as thermal interaction with the external environment, are explicitly modeled to ensure physical consistency and suitability for system-level integration.

The contribution presented in this work is primarily methodological and illustrates the modeling strategy, key assumptions, and design choices underlying the transition from a 0D approach under steady-state conditions to a dynamic 1D framework. The proposed model is intended as an evolving tool to support future experimental campaigns, control-oriented studies, and improved BoP design within r-SOC-based energy systems.

Keywords: Solid Oxide Cells, Reversible Operation, OpenModelica, Dynamic Modelling, Modular Framework

Poster Abstracts

Session B: Energy Conversion

Session B3: PEMFC

Direct formic acid fuel cell performance assessment with new hydrophilic electrodes and uniform reagent distribution system

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Abstract

Direct liquid fuel cells (DLFCs) represent a branch of fuel cell technology operating on liquid fuels. The diffusivity of liquids is 4 to 5 orders of magnitude lower than for gases. Therefore, DLFCs face more challenging mass transport conditions in the laminar flow regime. Consequently, significant effort is directed toward promoting convective transport and uniform reagent distribution, which is realized here by a novel mesh flow field design developed by the authors through a conceptualization process assisted by CFD simulations. This system is applied in this study to the direct formic acid fuel cell (DFAFC).

A critical aspect of DLFC operation is the management of CO_2 produced as a by-product at the anode. Bubbles initially emerge from the porous electrode to coalesce into slugs and flow along the channels. This phenomenon contributes to high pressure drops and restricts the mass transfer area between the channel and electrode, leading to bubble entrapment and blockage of the electrode area.

In this work, the authors investigate the effects of utilizing hydrophilic anodic electrodes within this novel mesh flow field design. The research tests the hypothesis that a hydrophilic electrode surface facilitates the detachment and removal of CO_2 bubbles and slugs, contributing to higher maximum power and current density of the system.

The study presents CFD simulation results comprising fuel concentration contours and flow distribution within the mesh flow field. These numerical results are accompanied by experimental verification, including current-voltage characteristics that demonstrate the differences in power and current densities between the conventional electrodes and the hydrophilic ones in a working DFAFC equipped with the mesh flow field design.

Keywords: Direct formic acid fuel cell, CFD simulations, hydrophilic electrode, mass transport, two-phase flow

Acknowledgements:
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Stress heterogeneities inside PEMFC stacks: a comparison between metal and carbon bipolar plates

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Abstract

Proton Exchange Membrane Fuel Cell (PEMFC) stacks are typically tightened to a nominal pressure which is often determined experimentally under specific operating conditions or estimated based on gas leakage criteria. However, the clamping pressure significantly impacts performance. The deformation state of individual cells within the stack is heterogeneous and the compression of the membrane electrode assembly depends on the design and structure of the bipolar plates which locally affect performance. Consequently, the nominal pressure depends on the stack components sizing, and operating regime. We have developed a model capable of evaluating the local compression state within a stack using a homogenization method. This model will ultimately link the clamping pressure to stack performance. In this study, we detail first the principles of the mechanical model, notably the measurements required to obtain the model parameters, then we present an application of the model to two different open-design stack configurations presenting the same active area: one with metal bipolar plates and one with carbon bipolar plates. Finally, we compare and discuss the mechanical behavior of the two stacks.

This work is conducted as part of the RealHyFC project, which is supported by the Clean Hydrogen Partnership and its members Hydrogen Europe and Hydrogen Europe Research under GA 101111904.

Keywords: PEMFC, mechanics, compression, bipolar plate, modelling

Electrochemical Impedance Spectroscopy and Relaxation Time Analysis for PEM Fuel Cells using Deep Learning

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Abstract

Polymer electrolyte membrane fuel cells (PEM-FCs) are complex electrochemical systems in which the coupled dynamics of proton transport, electrode kinetics, and multiphase transport give rise to overlapping, nonlinear loss processes that are challenging to understand and model. Electrochemical impedance spectroscopy (EIS) offers a powerful tool to probe these dynamics. However, the analysis and interpretation of EIS data are challenged by the presence of measurement noise, fluctuations in operating conditions, and the high dimensionality of the associated system parameters.

Our contribution presents a modular AI-based framework for generating synthetic EIS data corpora based on equivalent circuit models (ECMs), capturing a wide spectrum of parameter variations that are systematically organized into operating conditions and intrinsic system parameters (e.g., activation energies). In this regard, a well-established method to gain insights into the underlying electrochemical loss processes is the distribution of relaxation times (DRT) analysis, which is able to provide a structured mapping of impedance spectra features without requiring a priori knowledge.

To address the substantial volume of synthetic spectra required for a statistically robust analysis, deep learning concepts are integrated for efficient ECM classification. While deep feedforward networks serve as the primary models, alternative machine learning (ML) approaches and concepts are evaluated. Based on this methodology, we investigate the effects of data quality, measurement noise, and parameter variations on the reliability and accuracy of ECM identification across different ML paradigms and data modalities. Beyond facilitating high-throughput generation and labelling of synthetic datasets, the framework will offer a controlled platform for the systematic evaluation and refinement of data-driven analysis methods prior to their application in experimental EIS modelling.

Overall, the proposed approach establishes the basis for a reproducible and sustainable strategy for AI-supported equivalent circuit modelling which in the future shall also be applied to and validated on experimentally measured impedance data.

Keywords: ModVal2026, proton exchange membrane fuel cell, diagnosis, AI algorithms, electrochemical impedance spectroscopy, distribution of relaxation times.

Fluid dynamic and electrochemical interactions between flow field design and CCM properties in PEM fuel cells

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Abstract

Polymer electrolyte membrane (PEM) fuel cells represent one of the most promising solutions for the reduction of CO_2 emissions in the transport sector. In fact, they can be adopted in fuel cell electric vehicles (FCEV) for on board carbon free electrical current production. However, for PEM fuel cell technology to reach market maturity, optimizing performance thus reducing its costs is of course fundamental. In this context, computational fluid dynamic (CFD) analysis can represent a useful tool to enhance the understanding of reactants flow and distribution over the active area together with electrochemical reactions and losses distribution in the catalyst-coated membrane (CCM), which both strongly influence the overall performance of the cell. In this work an experimental and numerical comparative analysis of PEM fuel cell performance focusing on the combined effects of gas distributor geometry and CCM properties is carried out. Two different flow field configurations, consisting of parallel channels and a multi-pass serpentine distributor, are investigated as combined with two different CCMs characterized by different thickness. It results in four different configurations which are analysed integrating experimental polarization curve measurements with three-dimensional CFD simulations. The results highlight a strong cross-interaction between CCM properties and flow field design, indicating that their effects on PEM fuel cell performance are not independent. Flow fields promoting higher pressure gradients and enhanced under-rib convection partially mitigate the performance losses associated with thicker CCMs by improving reactant transport and water removal, while simpler configurations amplify mass transport limitations. These findings emphasize the need for a coupled optimization of electrochemical and fluid dynamic design parameters to achieve optimal cell performance.

Keywords: PEM fuel cell, CFD analysis, distributor geometry, CCM thickness

The Role of Transient Dynamics in PEM Fuel Cells: Polarization Hysteresis and Impedance Analysis

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Abstract

In the context of transitioning towards zero-emission mobility, proton exchange membrane fuel cells (PEMFCs) have emerged as a compelling technology for heavy-duty automotive applications. Steady-state modelling assumptions, although fundamental for performance predictions, lack time-dependent conditions that determine the initial state of degradation processes, as evidenced by hysteresis in polarization curves under real world operating conditions, i.e. voltage cycling. Such inaccuracy for the initial conditions for performance decays, has motivated to create PROMETHEUS: a transient-simulations extension of our 1D cell-scale MEA model [1]. The upgraded solver has been used to reproduce and highlight the relevant time-response mechanisms causing hysteresis. At the continuum-scale, membrane water sorption has been identified as the responsible process since it introduces a time-delay for the composition of the reactant mixture on the cathode gas compartment. At a lower scale, an oxygen mass transport and kinetics model for the oxygen reduction reaction (ORR) has been implemented based on the work of Sánchez-Ramos et al. [2]. This model considers the mesoscopic transport resistances through the ionomer and liquid water films. The surface oxidation/reduction of the platinum active sites is responsible for dynamic variation of the electrochemical active surface area (ECSA).

Moreover, the developed unsteady solver has been exploited to numerically simulate electrochemical impedance spectroscopy (EIS), which provides valuable information concerning the resistances of cell components, phenomena and regions of the polarization curves. In this context, we are using the EIS results to validate simulations vs. experimental measurements in the PEMTASTIC project. Specifically, Nyquist plots are used as diagnostics tool to guide modelling for physical and parametrizations needs, namely reparameterisation of reaction kinetics and local mass transport models.

References:
1. R.Vetter, J.O.Schumacher, Computer Physics Communications (2019), 234:223-234
2. Sánchez-Ramos et al., J. Electrochem. Soc. (2021), 168(12):124514

Acknowledgements: This work is funded by the Swiss State Secretariat for Education, Research and Innovation (SERI) and is part of the project PEMTASTIC, supported by the Clean Hydrogen Partnership and its members Hydrogen Europe and Hydrogen Europe Research under the Grant Agreement 101101433.

Keywords: ModVal2026, PEM Fuel Cell, Dynamics, EIS, Multiscale Coupling

Unified Microkinetic Modelling of Coupled Oxygen Reduction and Degradation Reactions in PEMFC Cathode Catalyst Layers

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Abstract

Proton exchange membrane fuel cells (PEMFCs) offer a promising pathway toward decarbonizing heavy-duty vehicle (HDV) transportation. Nevertheless, existing systems do not yet fulfil all HDV requirements, particularly regarding lifetime and energy conversion efficiency.

Within the cathode catalyst layer (CCL), the oxygen reduction reaction (ORR) constitutes the dominant source of activation overpotential, making it a critical factor governing cell performance. Concurrently, degradation reactions in the CCL cause progressive performance decline: carbon corrosion compromises the mechanical stability of the porous microstructure and may trigger structural collapse, while hydrogen peroxide acts as an important reactant in chemical membrane degradation reactions.

We present an electrochemical interface model that extends previous double layer descriptions [1] and unified ORR frameworks [2] by integrating a mass transport formulation capturing diffusion resistances across gas, ionomer, and aqueous phases. This bridges macroscale oxygen concentrations with a microkinetic description of surface reactions, including ORR [1], peroxide generation, and carbon oxidation [3]. The microkinetic model explicitly tracks time-depending coverages of surface-adsorbed intermediates, such as oxygen and hydroxyl species, enabling consistent coupling between reactions while accounting for site-blocking effects. Model parameters are calibrated against cyclic voltammetry and polarization curve measurements. The resulting framework yields insights for catalyst optimization and provides improved parameterization for cell-scale macrohomogeneous models.

References:
1. J. Huang et al., J. Phys. Chem. C, 120 (2016), 25, 13587–13595
2. J. Huang et al., Phys. Chem. Chem. Phys., 20 (2018), 17, 11776–11786
3. A. Kregar et al., J. Power Sources, 514 (2021), 230542

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Keywords: ModVal2026, PEMFC, Microkinetic Model, Degradation Reactions, Cyclic Voltammetry, Parameter Estimation

Impact of CO_2 and N_2 hydrogen dilution on PEMFC performance: A numerical study

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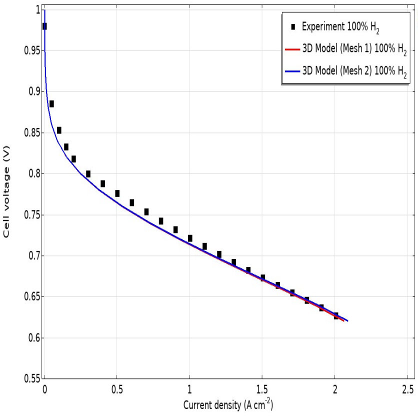
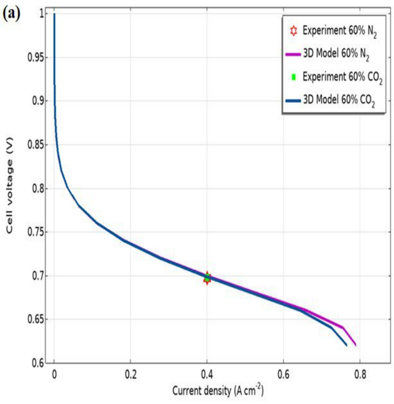
Abstract

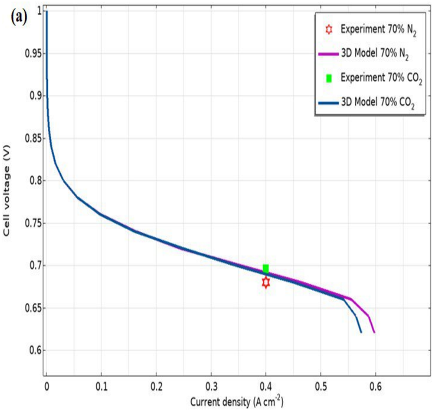
Proton exchange membrane fuel cells (PEMFCs) are promising devices for clean energy conversion; however, their performance can be significantly affected by hydrogen dilution in practical operating conditions. This work presents a three-dimensional numerical study of the impact of hydrogen (H_2) dilution with nitrogen (N_2) and carbon dioxide (CO_2) on PEMFC performance. The analysis focuses on polarization behavior, mass transport phenomena, and the role of key dimensionless numbers—Reynolds, Schmidt, and Peclet—within the anode gas channel. A steady-state 3D model was developed using COMSOL Multiphysics® and validated against experimental polarization data, showing good agreement. The results indicate that hydrogen dilution leads to a marked degradation of cell performance, with CO_2 dilution causing a more pronounced effect than N_2 dilution. At a current density of 0.4 A cm^{-2}, increasing the CO_2 concentration from 60% to 70% significantly increases the low-frequency resistance, highlighting severe mass transport limitations in the anode. Furthermore, the H_2/CO_2 mixture exhibits a 35% higher Reynolds number, a 21% lower Schmidt number, and a 19% higher Peclet number compared to the H_2/N_2 mixture, indicating faster flow velocities, enhanced diffusive transport, and stronger convective effects. A parametric study investigating the influence of inlet pressure, relative humidity, and reactant flow rate further demonstrates their critical role in mitigating dilution-induced performance losses.

These results provide valuable insights into the coupled transport phenomena governing diluted hydrogen operation and contribute to the optimization and validation of PEMFC models under realistic fuel conditions.

Keywords : PEM fuel cell; Hydrogen dilution; Numerical modeling; Mass transport.







MLP Neural Networks applied to PEMFC predictive degradation and control optimization

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Abstract

Proton Exchange Membrane Fuel Cells (PEMFCs) are promising energy conversion systems for transportation and stationary applications; however, their widespread deployment is hindered by performance degradation and durability issues under dynamic operating conditions. Accurate and real-time capable prediction of degradation and effective control strategies are therefore essential to enhance reliability and lifetime.

This work investigates the application of Multi-Layer Perceptron (MLP) neural networks for predictive degradation modeling and control optimization of PEMFC systems. The MLP model is trained using simulation data based on real drive-cycle scenarios to learn the nonlinear relationships between input operating variables and degradation indicators, enabling accurate prediction of voltage degradation and the Electrochemical Surface Area (ECSA) loss over time. The predictive models are then integrated into a control optimization framework with the objective of reducing degradation rates while maintaining performance (EDMS – Equivalent Degradation Minimization Strategy). This approach is compared with the conventional Equivalent Consumption Minimization Strategy (ECMS).

Simulation results demonstrate that the proposed MLP-based approach provides reliable degradation prediction and supports proactive control strategies. The findings suggest that MLP neural networks offer an effective and computationally efficient solution for predictive maintenance and advanced control of PEMFC systems.

Keywords: ModVal2026, MLP Neural Networks, Proton Exchange Membrane Fuel Cell, Predictive Degradation, EDMS

An elementary step-based reaction mechanism for carbon corrosion in PEMFCs

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Abstract

Hydrogen-powered Proton Exchange Membrane Fuel Cells (PEMFCs) are promising devices that are subject to several performance and durability issues requiring solutions. Some of the challenges relate to the catalyst layer (CL), which is composed of carbonaceous supports with Pt particles sitting on it, that are surrounded by several species in aqueous environment. To improve efficiency, durability and commercialization of PEMFCs, it is crucial to minimize the degradation of the carbonaceous material.

In the CL the carbon support undergoes oxidation (i.e., carbon corrosion), even though temperatures are below 100 °C, and that is due to the electrocatalytic aqueous environment, high applied potentials (0.60 – 1.4 V) and presence of Pt. When oxidising species (e.g. O2, H2O, H2O2, OH-, OH radicals) contact the carbon structure, CO and CO2 are formed and released, resulting in structural vacancies in the layer. This process causes the progressive degradation of the carbonaceous support.

In current literature, carbon corrosion is described through global reactions models featuring water and carbon support, e.g. C(s) + 2 H2O → CO2 + 4 H+ + 4 e–. These global reactions are simplifying a phenomenon that is much more complex and composed by several interconnected electrochemical reactions.

The carbon support is made of both amorphous and graphitised areas, among which the amorphous ones are more prone to oxidation. For this reason, soot has been chosen as model compound, in particular naphthalene. Further developments of this work may include the study of corrosion of a graphene layer, considering the presence of defects. Several possible reaction pathways have been analysed for the oxidation of naphthalene, reaction enthalpies and activation barriers have been calculated with Density Functional Theory (DFT) using Gaussian 16 with M06-2X method and SMD to address water solvation. Once known the energies of the structures, it is possible to evaluate the rate constants of reactions, also considering the applied potential.

The current work is formulating a reaction mechanism that includes such interconnected electrochemical reactions and their energy barriers in order to identify the rate determining steps in the overall carbon degradation process. From this study it is also possible to assess the impact that applied potential and Pt have on the carbon corrosion process, which is confirmed by experimental data.

This work is part of the BLESSED project funded by the European Union under Marie Sklodowska-Curie Actions and GA No. 101072578.

Keywords: Carbon Corrosion, DFT, Low T Fuel Cells, Catalyst Layer, Electrochemistry

Implementation and validation of a PEMFC mesoporous substructure electrode model into a 3D CFD-Code

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Abstract

Proton exchange membrane fuel cells (PEMFC) are promising for decreasing emissions in stationary and transport applications. To further improve their efficiency and long-term durability, a better understanding of the membrane electrode assembly behavior is necessary. The electrode support can be classified into low surface area (LSA) and high surface area carbons (HSA). Following those support types, the platinum (Pt) particles are primarily located on the carbon surface for LSA (Pt_{outer}) or inside pores for HSA (Pt_{inner}), leading to different cell behaviors regarding processes like the Pt-utilization. For a deeper understanding of those processes a performance modeling framework for analyzing the impact of Pt particle size distribution and carbon support structure was developed at Fraunhofer ISE [1]. Key features of this substructure model are the consideration of the Pt particle location allowing to predict specific loss mechanisms like proton accessibility issues for particles inside pores or ionomer poisoning and O_2 diffusion limitation due to densification of the ionomer film leading to a compact layer on particles on the carbon surface [1]. Part of this work is the model implementation into the CFD-Code FIRE M in cooperation with AVL. For the model validation, measured current and high frequency resistance data for an LSA and HSA carbon were used, which were obtained with a “Baltic ISE qCf Liquid Cooling high amp zero gradient” test cell (12 cm^2 active area) [2]. In addition, different inlet humidities were investigated with the aim of highlighting their impact on Pt-utilization as well as on the mass transport for particles inside pores and on the carbon surface. One finding was that the used HSA carbon showed strong performance loss with decreasing RH compared to the LSA carbon. This can be explained by inactive particles in the pores due to the lack of proton accessibility. By analyzing the separate polarization curves for the produced current of inner lying platinum, a stepwise activation of Pt_{inner} with higher RH could be observed, underlining the dependency of Pt-utilization from RH and the carbon support structure.

References:

1. Gerteisen D., Modeling the impact of Pt-particle position with respect of the C-support microstructure on PEMFC performance, European Fuel Cell Forum (EFCF) 2025, Lucerne, Schweiz, 1.-4. July 2025, doi: 10.24406/publica-5032
2. Schneider, P. et al. In-Situ Characterization of Cathode Catalyst Degradation in PEM Fuel Cells. Sci Data 11, 828 (2024). https://doi.org/10.1038/s41597-024-03662-w

Keywords: PEM fuel cell, 3D CFD, performance modelling, carbon support types

Innovative approaches to freeze/thaw cycling in PEM fuel cells: unveiling degradation mechanisms and multi-scale aging modeling

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Abstract

Freezing environments present a significant challenge for Proton Exchange Membrane Fuel Cells (PEMFCs), especially in automotive applications where rapid, energy-efficient start-up is critical. Mechanical degradation within the cells, triggered by repeated freeze/thaw cycles and cold start difficulties, which directly compromise system durability and performance are two key issues. Ice formation in bipolar plates, gas diffusion layers and catalytic layers causes delamination and accelerates degradation of the membrane-electrode assembly (MEA), drastically shortening its operational lifespan. Recent studies report a 2.4% loss in performance after only 3,000 freeze/thaw cycles, highlighting the urgent need to develop optimized cold start strategies that minimize energy costs, start-up time, and component degradation.

To tackle these challenges, the PEPR DuraSyS-PAC project adopts a collaborative approach designed to deliver practical solutions. As part of this initiative, LEPMI and CEA have developed a methodology that integrates advanced experimentation and modeling to pinpoint critical factors and validate robust mitigation strategies. In this work, we focus specifically on the experimental results obtained and the protocols established to characterize degradation mechanisms during freeze/thaw cycling.

Preliminary tests to assess the impact of freeze/thaw cycles on PEMFCs are conducted between -20°C and +10°C. The fuel cell undergoes several hundred freeze/thaw cycles out of operation of the fuel cell. The loss of performance, loss of ECSA, and increase in cell resistance are carried out after the break-in phase and during cycling to monitor any changes in performance. In addition, an in-depth study of materials and interfaces is underway to elucidate the underlying mechanisms. A dedicated experimental platform will enable passive hydrothermal cycles (without active gases) to be carried out, both *ex-situ* and *in-situ*, in order to stress the components and MEAs.

Keywords: Proton Exchange Membrane Fuel Cell, Freeze/thaw cycles, degradation mechanisms

Acknowledgement: This work has been supported by the French National Research Agency funding managed under the Plan France 2030 / reference ANR-22-PEHY-0002 (DuraSyS-PAC)

Two-phase flow simulation of multi-droplets motion in gas channel of polymer electrolyte fuel cells

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Abstract

Effective water management is a critical requirement for stable and high-performance operation of proton exchange membrane fuel cells (PEFCs). In this work, a three-dimensional volume-of-fluid (VOF) framework implemented using the openFOAM is employed to investigate two-phase flow in a PEFCs gas channel (GC), considering multiple liquid breakthrough inlets with different geometries. The gas diffusion layer (GDL) is modeled as a zero-dimensional liquid source, with some discrete breakthrough locations designed to represent heterogeneous water emergence at the GDL–channel interface. The simulations capture droplet growth, deformation, interaction, and detachment under imposed airflow (Fig. 1). The results show that some breakthrough geometries, such as triangular, acute angle towards the vertical wall of the GC, induce strong transverse and promote earlier detachment and enhanced drainage, whereas other geometries, such as circular or hexagonal openings, favor stable droplet growth and longer residence times. The study provides mechanistic guidance for GDL microstructure and flow-field design.

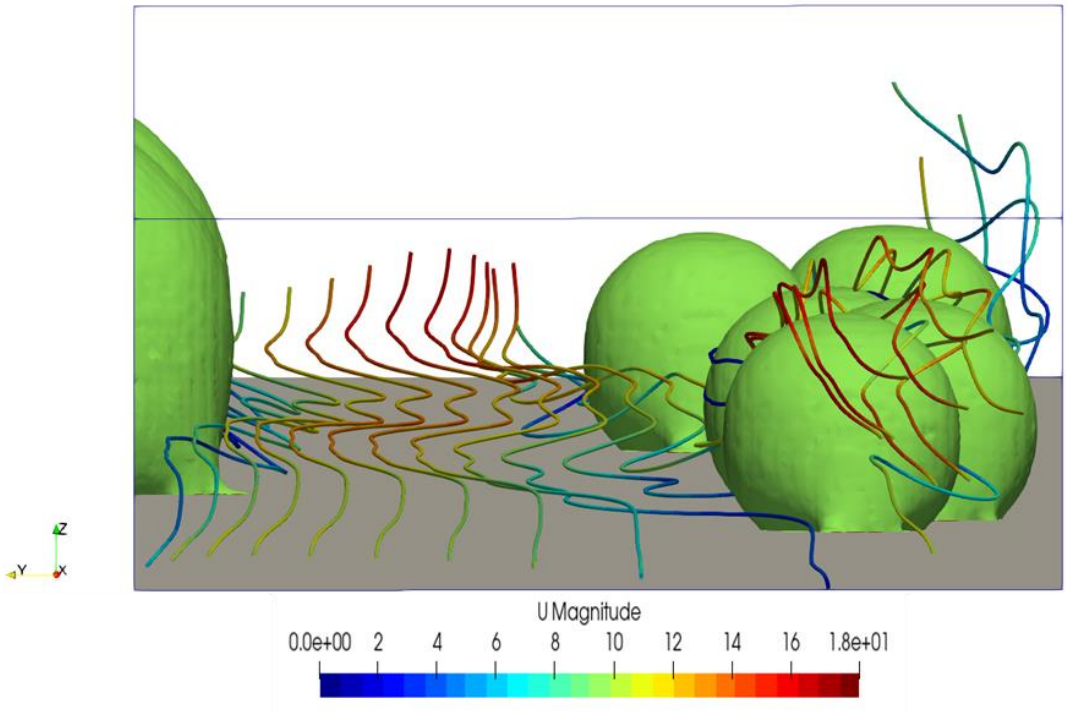

Fig. 1 View inside an PEFC GC, streamlines flow over the droplets

Keywords: Polymer electrolyte fuel cells, VOF, GDL surface, water management

Microstructure-Dependent Carbon Corrosion in PEMFC Cathodes under Accelerated Stress Testing

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Carbon corrosion of the catalyst layer supports in Polymer Electrolyte Membrane Fuel Cells (PEMFCs) is a key durability challenge. Under realistic operating conditions, multiple degradation processes occur simultaneously; therefore, it is difficult to disentangle the individual factors contributing to carbon corrosion and performance degradation. In this study, we investigated the influence of carbon support microstructure on stage-wise corrosion behavior and performance decay. To this end, we compared commercial Tanaka Kikinzoku Pt/C supported on Ketjen and Vulcan carbons with platinum loadings of 30 and 50 wt% under 20,000-cycle Accelerated Stress Test. Operando quantification via real-time CO_2 monitoring was used to determine the carbon loss at the cathode exhaust. This was correlated with electrochemical diagnostics, including Electro Chemical Surface Area (ECSA) measurements, polarization curves, electrochemical impedance spectroscopy with Distribution of Relaxation Times analysis, and Raman spectroscopy.

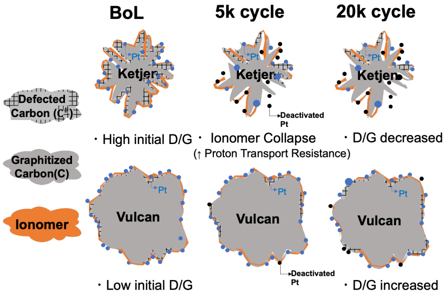

Figure 1. Support-dependent degradation schematic: Ketjen—early defect-rich carbon removal and ionomer degradation (↑ proton transport resistance, D/G ↓); Vulcan—gradual corrosion across cycles.

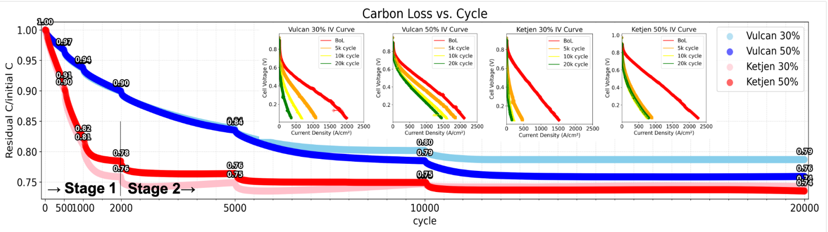

Figure 2. Operando carbon-loss evolution and polarization-curve decay during AST, highlighting distinct degradation trajectories between Ketjen and Vulcan despite comparable cumulative carbon loss.

In this study, we demonstrated that carbon microstructure was a key design parameter in PEMFC catalyst layers. We also showed that tuning defect density and porosity was critical for carbon durability while preserving proton transport related performance.

Reference:

1. J. Zhao et al., Journal of Power Sources 488 (2021) 229434
2. R. Borup et al., Chemical Reviews 107 (2007) 3904–3951

Keywords: Modval2026, Polymer Electrolyte Membrane Fuel Cell, Carbon Corrosion, Pt/Ketjen, Pt/Vulcan, Accelerated Stress Test

Optimizing the Range of a Fuel Cell Electric Vehicle with a genetic algorithm

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Abstract

Decarbonizing the transport sector is one of the promising ways to combat global warming and one which is already underway with the shift to electrified propulsion, synthetic carbon neutral fuels and hydrogen-based technologies. Fuel Cell Electric Vehicles (FCEV), as a combination of both hydrogen and electrified propulsion, could be part of this strategy, especially in heavy-duty or long-range passenger vehicles. Both system design and operating strategy have to be simultaneously optimized in order to improve system efficiency, weight and vehicle range. This can be done in the pre-design phase with a model-based approach and at later stages be experimentally validated. Here, a simplified vehicle model was created out of the combination of relevant component models and utilized to evaluate potential system configurations for a pre-design study. This was investigated further with a Monte Carlo parameter study, using Latin Hypercube Sampling (LHS) to generate the parameter combinations and an optimization of the system design and operating parameters utilizing the multi-objective Non-Dominated Sorting Genetic Algorithm II (NSGAII). The results of both optimization and parameter study were compared and analyzed in order to detect anomalies and potentially derive non-trivial connections or correlations. Both the model itself and the results will be the basis for further investigations in the iterative design-process. The model will be expanded and improved upon in future iterations and itself and its component models experimentally validated and potentially utilized in digital twins.

Keywords: ModVal2026, FCEV, System Model, System Optimization

1D-Degradation Models to Study PEMFCs

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The long-term reliability of PEMFCs remains a significant challenge, primarily due to degradation processes within the membrane and catalyst layers. This work consolidates key insights from our extensive research into developing degradation models for PEMFCs [1–9].

This presentation provides an overview of the semi-empirical and physics-based degradation models for Pt/C catalysts [1-3] and perfluorinated membranes [5-6] that we have developed over the past decade.

The models enable the prediction of chemical degradation in polymer electrolytes within both the membrane [5] and catalyst layers, as well as Pt oxidation and dissolution. One specific model predicts the mechanical stability of Nafion membranes under cycling relative humidity [8]. Additionally, several of the developed models are integrated with a commercial CFD code, facilitating the study of localized degradation effects in real-world fuel cells [4, 7].

The Pt/C catalyst degradation model has been applied to assess Pt lifetime under various accelerated testing protocols and to calculate Pt/C lifetime under voltage cycling conditions [1-3].

The developed models serve as powerful tools for understanding and mitigating degradation processes in PEMFCs, thereby contributing to their improved reliability and durability. These advancements play a crucial role in accelerating the adoption of PEMFCs in sustainable energy applications.

References:

1. L. Karpenko-Jereb, V. Kovtunenko. Inter. J. Hydrogen Energy. 48 (2023), 41, 15646–15656.
2. V. Kovtunenko, L. Karpenko-Jereb. Technologies. 80 (2021) 1-10.
3. V. Kovtunenko, L. Karpenko-Jereb. J. Power Sources. 493 (2021), 229693
4. C. Fink, S. Gößling, L. Karpenko-Jereb, P. Urthaler. Fuel Cells. 20 (2020), 431-452.
5. L. Karpenko-Jereb, C. Sternig, C. Fink, V. Hacker, A. Theiler, R. Tatschl. J. Power Sources 297 (2015), 21452, 329-343.
6. L. Karpenko-Jereb, C. Sternig, C. Fink, R. Tatschl. Inter. J. Hydrogen Energy. 41 (2016) 13644-13656.
7. C.Fink, L. Karpenko-Jereb, S. Ashton. Fuel Cells. 16 (2016), 4, 490–503.
8. A.Theiler, L. Karpenko-Jereb. 40 (2015), 31, 9773-9782
9. L. Karpenko-Jereb, P. Innerwinkler, A.-M. Kelterer, C. Sternig, C. Fink, P. Prenninger, R. Tatschl. Inter. J. Hydrogen Energy 39 (2014) 7077-7088.

Keywords: Polymer Electrolyte Fuel Cells, Modelling, Degradation & State of Health, Virtual Sensors, Accelerated Stress Test

Hybrid DEM-VoF Multiphase Model for Microchannels of Electrochemical Devices

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Abstract

In proton exchange membrane (PEM) electrolyzers and in low-temperature PEM fuel cells, the reaction process leads to the formation of two-phase flow in microchannels. Therefore, the secondary phase needs to be removed effectively to ensure high performance and longevity of the device. A deeper understanding of this removal process is needed to optimize the cell design of electrochemical devices.

Computational fluid dynamics (CFD) is widely used to investigate multiphase flow. Because different flow regimes ranging from disperse to continuous flow occur in the microchannels of such devices, the selected multiphase model needs to capture different length scales. The volume of fluid (VoF) method requires high mesh resolution to accurately capture the interface between the phases. Consequently, for disperse flow, this method incurs a high computational cost. In contrast, the Euler-Euler model might be computationally more efficient but is only applicable to the disperse phase, so it cannot capture the wide range of length scales present in the system. To bridge this scale gap efficiently, hybrid models have been developed that use different model equations depending on the local flow topology. In literature, the combination of the Euler-Euler model for the disperse phase with a VoF model for large interfaces is the most common. While effective for large-scale processes, these models neglect surface tension in the disperse phase, preventing accurate prediction of the detachment dynamics of droplets or bubbles in microchannels.

In this contribution, we propose using a hybrid model that couples a discrete element method (DEM) for the disperse phase and its transition to large structures with a VoF method for large structures. The DEM is an extension of the Euler-Lagrange framework to finite-size particles. This DEM-VoF approach is intended to capture detachment dynamics accurately and, as a result, to enhance prediction of multiphase flow in microchannels. First, we develop the DEM component for modeling detachment dynamics and validate it by comparison to experimental data from literature. Next, we describe the coupling strategy between VoF and DEM and demonstrate the application of this methodology. With this approach, a more physical and efficient simulation for two-phase flow in microchannels of electrochemical devices is possible.

Keywords: ModVal2026, multiphase, simulation, proton exchange membrane fuel cell, proton exchange membrane electrolysis

The influence of transport porous layer wettability on Direct Formic Acid Fuel Cell performance

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Abstract

Direct formic acid fuel cells (DFAFCs) are a type of proton exchange membrane fuel cell supplied with liquid formic acid (FA) and air. They are known to be promising candidates as low-emission power supplies. However, the ongoing electrochemical reaction, on the anodic side of DFAFC, produces CO_2. This phenomenon results in the formation of two-phase flow, primarily in the Taylor (slug) regime. Consequently, it obstructs FA access to the catalytic layer of the fuel cell, thereby decreasing its efficiency.

CO_2 bubble behavior can be altered by a change in the porous transport layer (TPL) wettability. This work investigates the effect of carbon cloth (CC) wettability on the performance of DFAFC. Both numerical and experimental methods have been employed to thoroughly examine the presented phenomenon.

An effective method of CC hydrophilization has been proposed. Moreover, different methods of catalyst ink deposition on it have been compared. IPA, EtOH, and water-based inks are investigated in terms of particle size in dispersion and their rheological properties. To further compare the influence of the wettability of TPL on DFAFC performance, current-voltage and power density characteristics have been investigated.

Subsequently, Computational Fluid Dynamics has been used to investigate the influence of carbon cloth contact angle on flow hydrodynamics. A simplified approach to CC modeling has been adopted. Each tow has been approximated as an ellipse swept through a sinusoidal path. Porosity in each tow between single carbon fibers has been neglected. Characteristic properties such as FA concentration distribution and two-phase flow behavior have been compared for different CC contact angles. Outcomes for the proposed geometry of TPL have been equated with the isotropic porous zone approach.

Furthermore, a high-speed camera has been used to visually study the influence of TPL wettability on CO_2 bubble morphology. The OpenCV® package for image analysis has been used to collect data from acquired images in order to quantitatively compare TPL with different contact angles.

This work emphasizes the influence of CC wettability on the two-phase flow in DFAFC as well as proposes a method of numerically modeling its effect. Novelly fabricated MEA registered a 22% increase in peak cell power density and a 14% increase in maximum current load compared to the previously used MEA.

Keywords: Direct Formic Acid Fuel Cell, Transport porous layer, Wettability, CO_2 bubbles, Volume of Fluid.

Model-Based Reduction of the Required Validity Space of Electrochemical Models for Efficient Testing

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Abstract

Electrochemical systems are set to play a role in decarbonizing the economy. These systems are increasingly complex, and, combined with their novelty, make modelling and testing challenging. This is why we are developing an integrated testing methodology improving the parameter identification for the simulation models needed to develop those new systems, as outlined in [1]. This method targets component or sub-system level models in a three-part strategy leveraging the information contained within the investigated model, highly automated testing equipment and recent advances in optimization techniques. First, we build a model of the future power system application that our target model will be running in. This application model is used to find the required validity space for the target model. Second, we combine information from the target model and the testing equipment to design an optimal set of experiments, similarly to the method described by Goshtasbi et al in [2]. Third, once the experiments start, we use a Bayesian optimization technique to steer the upcoming and pending experiments using the freshly obtained information from the past experiments. This contribution focuses on the first part.

The methodology is illustrated by applying it to an electric deep drilling machine that is being equipped with a fuel cell system. Here, the target model is the model of the Toyota fuel cell system, and the application is the complete battery-fuel-cell-hybrid drivetrain powering the deep drilling machine. All models are implemented in Modelica. The model for the Toyota fuel cell system whose parameters need to be identified is implemented. Next, the model for the entire power system is set up, including the battery, electric circuitry, cooling systems and fuel tanks. Using a load-profile describing the machine's power demand over different operating days, combined with corresponding ambient conditions profiles, we can deduce the operating range that the fuel cell system model needs to cover. This is done through analysis of the interface of the fuel cell system with the rest of the application model. Using the space spanned by those results, experiments are designed to capture the relevant areas. These experiments are performed on a single Toyota fuel cell system. Using the results, the model parameters are updated. In this work, we show that capturing the exact operating range of the target model simplifies the complex parameter identification task, completing one of the three blocks of our integrated testing methodology.

References:
[1] Oswald, T., Weiss, L., and Wensing, M., SAE Technical Paper 2024-01-4322
[2] Alireza Goshtasbi et al 2020 J. Electrochem. Soc. 167 044504 and 167 044505

Keywords: ModVal2026, Fuel Cell Hybrid Systems, X-iL testing, DOE, parameter identification

Influence of the Cathode Catalyst Material Selection on the Cathode Gas Transport Processes in PEMFC

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Abstract

In order to achieve high power densities with Polymer Electrolyte Membrane Fuel Cells (PEMFC) an adequate supply of reactant gases to the Three Phase Boundary (TPB) of the electrode layers is mandatory. The ability to supply oxygen to the TPB and remove product water depends on the microstructures of the chosen Gas Diffusion Layer (GDL) and the Cathode Catalyst Layer (CCL). When producing the CCL, type and content of ionomer, carbon support and catalyst can be varied in wide ranges, resulting in different electrode microstructures varying in performance.

In this contribution, PEMFCs with different CCL compositions but identical loadings are compared regarding gas diffusion in GDL and CCL. A combination of Limiting Current Measurement (LCM) and Electrochemical Impedance Spectroscopy (EIS) is applied.

To characterize and quantify the gas transport losses, EIS and a subsequent Distribution of Relaxation Times (DRT) analysis are performed to deconvolute the different loss processes in the cells [1]. Furthermore LCMs are applied to separate gas diffusion contributions of CCL and GDL [2], providing access to the gas diffusion resistances of the different CCLs. This enables a physiochemically motivated Equivalent Circuit Model (ECM), which models CCLs and GDL separately. Whereas the common Warburg Element is applied to cover gas diffusion in GDL and MPL [1], the gas diffusion in the different CCLs was integrated in the Transmission Line Model (TLM) representing the coupling of gas and ionic transport by the charge transfer reaction in the CCL [3]. Fitting this TLM to measured spectra provides quantitative values for the gas transport resistance in the ECM for different CCLs, making a direct comparison of different CCLs possible. In this contribution, the gas diffusion resistances of different CCLs are evaluated for a variety of operating conditions and will be correlated with microstructural features of these layers.

References:

[1] Heinzmann, M., et al. (2018). "Advanced impedance study of polymer electrolyte membrane single cells by means of distribution of relaxation times." Journal of Power Sources 402: 24-33.

[2] Spingler, F. B., et al. (2017). "Investigating fuel-cell transport limitations using hydrogen limiting current." International Journal of Hydrogen Energy 42(19): 13960-13969.

[3] Dierickx, S., et al. (2019). "Advanced impedance model for double-layered solid oxide fuel cell cermet anodes." Journal of Power Sources **415**: 69-82.

Keywords: CCL Composition, Impedance Modeling, Limiting Current, Gas Transport Characterization

PEMFC Local Fault Identification by Magnetic Tomography and Deterministic Optimization

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Abstract

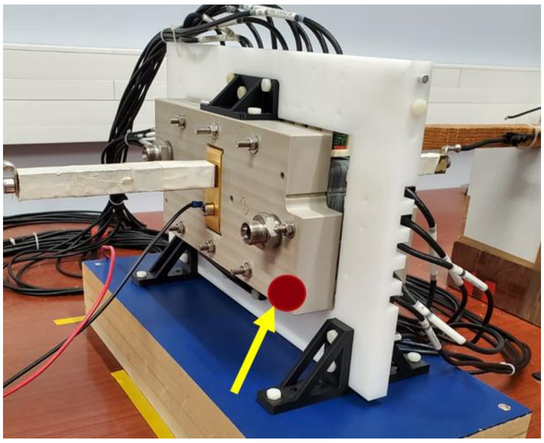

Figure 1: FC-Stack and placed fault location indicated with red dot and yellow arrow.

A proton exchange membrane fuel cell (PEMFC) is an electrochemical converter that represents an environmentally friendly alternative to fossil fuels. A PEMFC stack consists of several cells connected in series, whose aging is a major problem and requires accurate diagnosis to adjust the stack control and operation, and thus optimize its reliability and lifetime. Magnetic tomography (MT) is a non-invasive diagnostic method that can be used to obtain local current densities $\boldsymbol{J}$ and local material properties inside FC-stacks. In this method, the external magnetic field $\boldsymbol{B_m}$ created by the current flowing through the stack is measured using magnetic field sensors placed around it (see Figure 1). A numerical model is then inverted to determine the current density distribution. While most studies propose methods for determining current densities, the originality of our approach lies in the direct identification of local resistivities ρ_{local}, using a nonlinear optimization algorithm. The resistivity is a scalar physical property, simplifying the fault identification compared to a 3D-vector quantity such as local current densities. To validate the capability of our algorithm, a test campaign was conducted using a purely conductive mockup of a stack (see Figure 1). The latter is consisting of 40 cells composed only of gas diffusion layers (GDL) and bipolar plates. This configuration allows introducing controlled faults within the stack by placing a localized insulating layer measuring a few cm². By applying a current to the stack, the magnetic field around it, as well as cell voltages and the stack voltage can be measured. Based on this data (current, voltage, and magnetic field), our algorithm is able to identify and localize the defect in the stack. The robustness, accuracy, and detection capability of our algorithm will be compared to the commercial S^{++}® device and discussed based on various case studies.

Keywords: ModVal2026, proton exchange membrane fuel cell, magnetic tomography, non-invasive diagnostics

Microscopic Mechanical Models for PEM Compared to Real Cell Deformations

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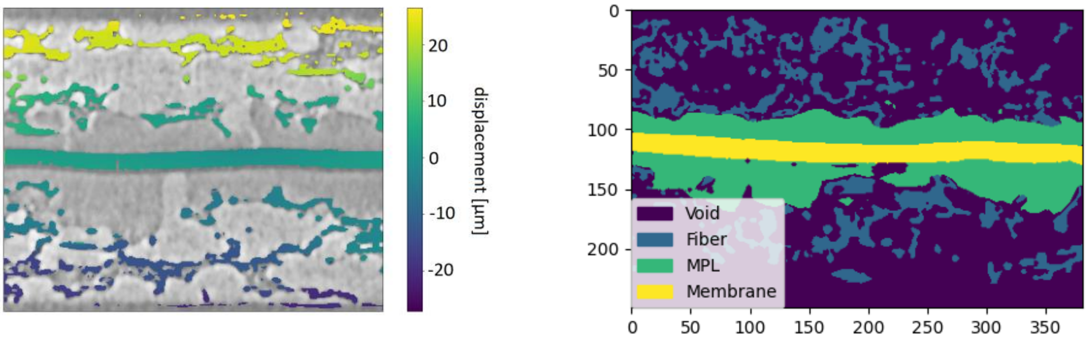
Abstract

During the cell assembly of a PEM fuel cell, mechanical compression is applied to ensure sufficient electrical contact between components, placing significant mechanical demands on the gas diffusion layer (GDL), the microporous Layer (MPL) and the membrane. As the most compressible components within the cell, the GDL accommodates the majority of the deformation, and its mechanical response largely determines the stress applied to the membrane.

Microscale finite element (FEM) models of the GDL have been proposed to describe the mechanical behavior of the GDL and the membrane and have been shown to reproduce the macroscopic stress–strain response observed in compression experiments. In this work, X-ray computed tomography (CT) imaging is used to experimentally investigate the microscopic deformation inside a cell like setup consisting of a Nafion membrane clamped in between two GDLs and MPLs under compression. The CT images are segmented with a trained AI model to identify the individual cell components and to enable the local displacement tracking of the components. Quantitative deformation parameters are extracted and are compared with the displacements predicted by the microscopic model. Based on these parameters, the accuracy of the model and the validity of the underlying modeling assumptions are discussed.



Figure, left: Microscopic displacement of a GDL, MPL, Membrane stack obtained by digital volume correlation of CT images. Figure right: Segmentation of CT images into the different cell components.

Keywords: Fuel Cells, Electrolysers, PEM, Mechanics, AI Segmentation

Ex situ small angle neutron scattering study of water uptake in hydrocarbon based catalyst layers

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Abstract

While hydrocarbon (HC) ionomers can compete or outperform current perfluorosulfonic acid (PFSA) ionomers in dry operating conditions of polymer electrolyte fuel cells, they are prone to flooding at high humidity operation conditions. The reason is not clear but difference in ionomer distribution and water saturation depending on the ionomer chemistry most probably play a role. Unlike PFSA, which likely coats the catalyst surface, HC ionomers may penetrate carbon nanopores, improving hydration and performance. The ionomer content may also influence pore accessibility to water.

Small angle neutron scattering measurements were conducted at the D22 beamline of the Institut Laue-Langevin (ILL, Grenoble, France) on catalyst layer powders prepared with two ionomer types (HC and PFSA), each at two different loadings relative to the catalyst mass. The samples were investigated at relative humidity (RH) levels of 0, 50, 70, 80, and 95% using both H_2O and D_2O, with an additional 100% RH measurement with D_2O to ensure condensation. For reference, the bare catalyst and each ionomer were measured also separately.

Preliminary results indicate that the catalyst layer with hydrocarbon (HC) ionomer exhibits significantly greater water-induced adsorption compared to the perfluorosulfonic acid (PFSA) ionomer. This is evidenced by the pronounced decay in low-Q intensity observed in the HC-based catalyst layer, suggesting that a substantial portion of the largest pores becomes filled at high relative humidity (RH).

Keywords: Polymer electrolyte fuel cell, catalyst layer, liquid water, ionomer

Poster Abstracts

Session B: Energy Conversion

Session B4: PEMWE

Evaluating the Validity of In Situ Reference Electrode Measurements in PEM and AEM Water Electrolysers

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Abstract

In situ reference electrodes are valuable tools that enable the deconvolution of the anode and cathode contributions to performance loss in water electrolysers. For many reference electrode techniques, however, the validity of the half-cell potential and impedance measurements is debated. In this work, a reference electrode in contact with the membrane at the edge of the active area was applied in both proton and anion exchange membrane cells. Experimental results were used in conjunction with a 2D model to validate the edge-type configuration in the proton exchange membrane system. It was found that by correcting for ohmic losses using impedance spectroscopy at each current/potential point, the position of the reference electrode due to anode-cathode misalignment could be accounted for. Through this work, we establish best practice guidelines for experiments with edge-type reference electrodes and interpreting the half-cell data generated. It was possible to measure the impact of platinum loading on cathode kinetic and mass transport losses using this technique. Reliable impedance measurements were also demonstrated for an anion exchange membrane electrolyser. This three-electrode cell technique presents a robust platform for studying kinetic and mass transport performance losses in both proton and anion exchange membrane water electrolysers.

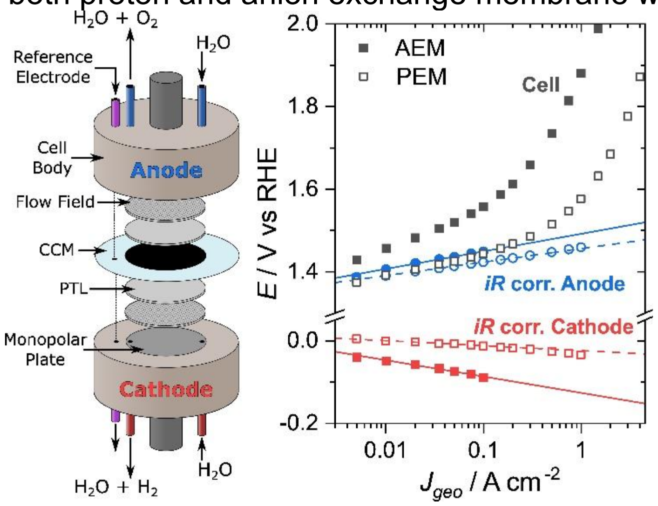

Figure: Left: Diagram of three-electrode cell with edge-type reference electrode. Right: Full and half-cell polarisation curves from the three-electrode cell for both AEM and PEM electrolyser systems.

Keywords: ModVal2026, three-electrode cell, AEM, PEM, water electrolysis

Poster Abstracts

Session B: Energy Conversion

Session B5: AEMWE

Model-Based Design Engineering for Industrial AEM Electrolyzer Stacks Using Coupled 1D–3D Multiphysics Models

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Abstract

Industrial scale-up of AEM electrolyzer stacks is often limited by long experimental iteration cycles and the difficulty of translating stack-level measurements into actionable design choices (flow-field, contacting, compression, thermal and mass-transport management). We present a multi-fidelity, model-based design engineering workflow that couples a fast physics-based 1D model with a high-resolution 3D COMSOL multiphysics model to accelerate design decisions and validation at Gen-Hy Cube.

The 1D model is calibrated on polarization data using robust parameter identification, enabling rapid generation of operating maps and sensitivity rankings (e.g., contact/ohmic contributions, flow-dependence, and thermo-electrochemical coupling). These reduced-order outputs define the design space and identify priority levers before hardware iterations. The calibrated parameter set is then transferred to a 3D COMSOL model to resolve local gradients (current density, temperature, concentration/gas distribution) and quantify geometry-driven dispersion, providing mechanistic explanations behind observed performance spreads.

Finally, the workflow is used to quantify the impact of **interfacial/contact resistance** through **parameter identification** on experimental polarization data, and to propagate these calibrated electrochemical parameters into a reduced-order 3D COMSOL representation to assess **local gradients and dispersion** under representative operating conditions. Based on the model outputs, we define a validation plan consisting of **dedicated tests that isolate contact-resistance effects** (controlled compression/contacting, identical MEA batches, and repeated operating points) to reproduce the predicted performance deltas. In parallel, we propose **monitoring indicators** suitable for industrial testbenches (e.g., EIS-derived ohmic contribution, voltage mapping/cell-to-cell dispersion, thermal signatures, and trend-based alarms) to secure operation and accelerate design iterations.

Keywords: AEM electrolysis, model-based design engineering, multi-fidelity modelling, COMSOL, stack scale-up, validation, operating maps

A numerical and analytical model to predict the bubble surface coverage in water electrolysers

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Abstract

Bubbles adhered to electrode surfaces during water electrolysis significantly reduce electrolyser performance by increasing ionic transport resistance in the electrolyte and by lowering the active electrode surface area. Thus, bubble surface coverage is an essential parameter in modelling electrolysers. In water electrolysis, bubbles nucleate within sub-micron-scale surface crevices, where high supersaturation of dissolved gas drives early-stage growth. Despite the well-documented influence of surface roughness and crevice size distributions in boiling phenomena, their role in gas-evolving electrochemical systems remains largely underexplored.

In this work, we develop a combined numerical and analytical framework that links the sub-micron-scale distribution of crevice sizes on the electrode to the macroscopic bubble surface coverage. Using a power-law for the crevice size distribution, consistent with treatments in the boiling literature, we conduct numerical simulations across a range of crevice size distributions (varying size ranges, number density, and positions along an electrode), concentration boundary layer thicknesses, and current densities to obtain the bubble surface coverage. We derive an analytical model using a one-dimensional transport equation for dissolved gas and validate it against numerical results to confirm its predictive capability at low surface coverages. This model also explains experimentally observed trends in surface coverage reported in the literature, providing a mechanistic link between crevice size distribution, surface coverage, current density, and supersaturation.

Keywords: Bubble surface coverage, alkaline water electrolysis, analytical and numerical model

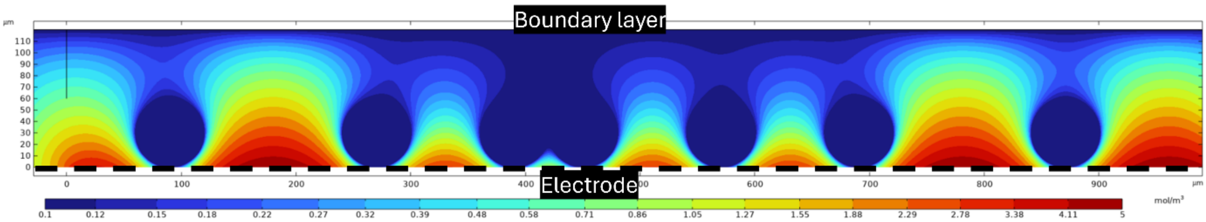

Figure 1. A section of the electrode from the simulation carried out at a current density of $90\ [\mathrm{A/m^2}]$ showing the dissolved gas concentration (in colour) contour for one instance of the crevice size distribution and concentration boundary layer thickness. The bubbles adhered to the electrode surface are represented with regions with a saturation concentration of $0.1\ [\mathrm{mM}]$ next to the electrode.

Modelling of Mass Transport Limitations in Mixed Wetting Gas Diffusion Electrodes

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Abstract

The chlor-alkali electrolysis is an exceedingly important process utilized on industrial scale for the coupled production of chlorine and sodium hydroxide from NaCl solutions with a total demand for electrical energy of 195800 GWh in 2017 [1]. This process usually relies on gas diffusion electrodes for the oxygen reduction reaction (ORR) at the cathode.

$$O_{2,(aq)} + 2H_2O + 4\,e^- \rightarrow 4\,OH^-$$

The performance of these electrodes relies on electrolyte distribution in the electrode. The ORR takes place at the electrode surface, which is in contact with electrolyte. Mixed-wetting materials are utilized, which consist of an electrically conducting material, which usually catalyses the ORR, and a hydrophobic material to inhibit flooding of the electrodes. In the case of chlor-alkali electrolysis, this can be achieved by utilizing a silver-based GDE, which employs polytetrafluorethylene (PTFE) as the hydrophobic agent [2]. In this work, a lattice Boltzmann model for the simulation of dissolved O_2 and mass transport limitations of hydroxyl-ions inside of the flooded GDE, is presented. The lattice Boltzmann method is chosen due to its capability to treat complex geometries and parallel computing affinity. A single relaxation time (SRT) model with D2Q5 and D3Q7 lattice discretisations are chosen, which is sufficient to describe the governing diffusive transport in the electrolyte phase. Simulations are performed for 2D test-cases and the real structure of a mixed-wetting GDE, obtained by FIB-SEM analysis, is employed for the full-scale 3D simulations. Figure 1 shows three-dimensional GDE structure, used for the full-scale simulations.

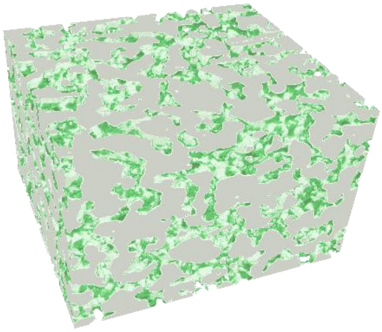

Figure 1: 3D GDE structure containing silver (white) and PTFE (green).

In further studies, a phase-field based LBM description of electrolyte imbibition is to be implemented to calculate the full electrolyte distribution from first principles

Keywords: Mixed Wetting Gas Diffusion Electrode, Lattice Boltzmann Method

[1] J. Kintrup, M. Millaruelo, V. Trieu, A. Bulan, and E. S. Mojica, “Gas Diffusion Electrodes for Efficient Manufacturing of Chlorine and Other Chemicals,” *Electrochem Soc Interface*, vol. 26, no. 2, pp. 73–76, Sep. 2017, doi: 10.1149/2.F07172if.

[2] F. Bienen *et al.*, “Investigating the electrowetting of silver-based gas-diffusion electrodes during oxygen reduction reaction with electrochemical and optical methods,” *Electrochemical Science Advances*, vol. 3, no. 1, pp. 1–12, Feb. 2023, doi: 10.1002/elsa.202100158.

Multiphysics model describing the performances of AEM electrolyzer cell

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Abstract

Anion Exchange Membrane Electrolyzers (AEMWE) represent a promising technology for decarbonized hydrogen production, offering advantages such as the use of non-precious metal catalysts and the absence of fluorinated membranes. For design and optimization purposes, it is crucial to understand the various physical phenomena occurring within an AEMWE cell and to model them using a numerical tool capable of simulating operations under different conditions. Building on its experience with PEM fuel cell and PEM water electrolyzer codes, CEA has developed both 1D and 2D versions of a code to simulate the operation of a dry cathode AEM electrolyzer cell. This code integrates fluidic and thermal models with electronic, ionic, and electrochemical models. Compared to PEM codes, the AEM code is more complex due to the asymmetric nature of the underlying physics and the involvement of new phenomena.

On the anode side, oxygen is produced and dissolves in the liquid until saturation, leading to the formation of bubbles that move through the mesh grid toward the outlet. Two-phase flow is modeled using the Darcy approach, considering the real geometry for permeability (both absolute and relative) based on 3D images and GeoDict software. Additionally, KOH is present in the water and plays several roles that are not yet fully understood. It enhances ionic conduction in the catalyst layer and potentially influences electrochemical kinetics (see the companion presentation by Bretillon et al.). We consider the configuration with absence of ionomer in the active layer, as the distribution of hydroxide ion flux from the membrane to the liquid solution and ionomer remains unclear and is still under investigation. The electrochemistry is modeled using the Butler-Volmer equation, accounting for the effect of bubbles on the electrochemically active surface area (ECSA).
On the dry cathode side, the real situation has been simplified by neglecting the presence of liquid water and KOH, focusing instead on hydrogen and vapor flux. The electrochemistry is modeled using the classical Butler-Volmer equation.
Within the membrane, the fluxes of oxygen and hydrogen are modeled using dissolution and diffusion laws. Ionic transport in both the membrane and the cathode ionomer is modeled using effective conductivity.
The code is able to provide polarization curves and remains now to be calibrated.

Keywords: ModVal2026, Anion Exchange Membrane Electrolyzer, Multiphysics model

Investigation of ionomer nature and pH roles on HER and OER in AEMWE using RDE for model calibration

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Abstract

Anion Exchange Membrane Water Electrolysis (AEMWE) has been increasingly studied for the past few years because it combines advantages of two existing technologies, namely alkaline water electrolysis (AWE) and proton exchange membrane water electrolysis (PEMWE). Green hydrogen is thus produced using non-PGM metals and non-fluorinated membranes with a higher performance than AWE. However, there is still room for improvement in terms of system efficiency and durability. Some phenomena occurring within the electrolysis cell are yet to be fully understood in order to optimize this type of electrolysis. For instance, the presence of KOH at the anode adds a supplementary pathway for conducting hydroxide ions through the catalyst layer compared to PEMWE. Although it is now clear that the use of KOH as electrolyte enhances AEMWE performance, its role is not fully explained yet. Moreover, some previous studies highlighted the importance of the ionomer nature, as using a proton-conducting ionomer such as Nafion enhances the AEMWE performance. This effect is yet to be understood, as well as the impact of local pH on the reactions' kinetics.

Hydrogen evolution reaction (HER) at the cathode and oxygen evolution reaction (OER) at the anode are not well-understood in AEMWE when using non-Platinum group metals (non-PGM) metals. A kinetic study of these two reactions in an alkaline environment could help to improve our knowledge of the mechanisms involved, for instance by measuring kinetic parameters such as the anodic and cathodic exchange current densities (i_0) and Tafel slopes obtained with those materials. These kinetic values influence the electrolysis performance and can be determined using a Rotating Disk Electrode (RDE). Non-PGM catalysts with either Nafion (H^+ conductive ionomer) or Aemion (OH^- conductive ionomer) are tested in order to highlight the impact of the nature of the ionomer on performance. These results aimed to provide insightful data to feed AEM models such as the Europium 1D and 2D Multiphysics model (see the presentation by Serre et al.) with experimentally based kinetics parameters. In addition, it intends to improve our understanding on the influence of the local pH on the HER and OER kinetics.

Keywords: ModVal2026, anion exchange membrane electrolyser, rotating disk electrode

Process Modelling of High-Pressure Alkaline Electrolysis, Syngas Generation, Methanol Synthesis, and Cost Estimation

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Motivation

Power-to-Methanol (PtM) enables chemical storage of renewable electricity while utilizing CO_2 as a feedstock, positioning it as one of the most promising routes toward carbon-neutral fuels and chemical circularity[1]. Methanol is a liquid energy carrier compatible with global transport and chemical infrastructure[2], which is usually produced from fossil-based syngas consisting of $CO/CO_2/H_2$. To make the methanol green, syngas must be generated from green H_2 and biogenic CO_2 via an intermediate step, i.e. reverse water-gas-shift (RWGS) reactor. Alkaline water electrolysis (AEL) is the most commercially mature and cost-effective technology for green hydrogen production. However, pressurized operation introduces non-linear trade-offs between reduced compression costs and increased internal electrochemical losses, especially at high currents or elevated pressures[3,4]. To address these challenges, this work establishes a comprehensive Aspen Plus® modelling and techno-economic framework that quantifies the influence of key operating parameters and identifies optimal conditions for efficient and economically viable high-pressure AEL-based PtM systems.

Methodology

Detailed AEL model is developed in Aspen Plus. This detailed AEL module is integrated with two PtM pathways:

(1) RWGS + syngas conditioning + methanol synthesis, modeled using literature-based RWGS equilibrium and validated methanol synthesis reaction kinetics;

(2) Direct CO_2 hydrogenation, modeled using validated methanol synthesis reaction kinetics.

Both routes are constructed in a comparable steady-state simulation framework in Aspen Plus® as shown in Figure 1, A systematic parameter study is performed varying AEL pressure, temperature, and current density to assess the influence on key performance

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[1] Kiss et al. (2016), Novel efficient process for methanol synthesis by CO_2 hydrogenation.

[2] M. Bertau et al. (2014), Methanol: The Basic Chemical and Energy Feedstock of the Future.

[3] Abdin et al. (2017), Modelling and simulation of an alkaline electrolyser cell.

[4] M. Sánchez Delgado (2019), Desarrollo y validación de un modelo para la simulación de sistemas de electrólisis alcalina para la producción de hidrógeno a partir de energías renovables.

indicators: hydrogen cost, system efficiency, methanol yield, and overall energy demand. The net production cost (NPC) of methanol is calculated consistently for both routes.

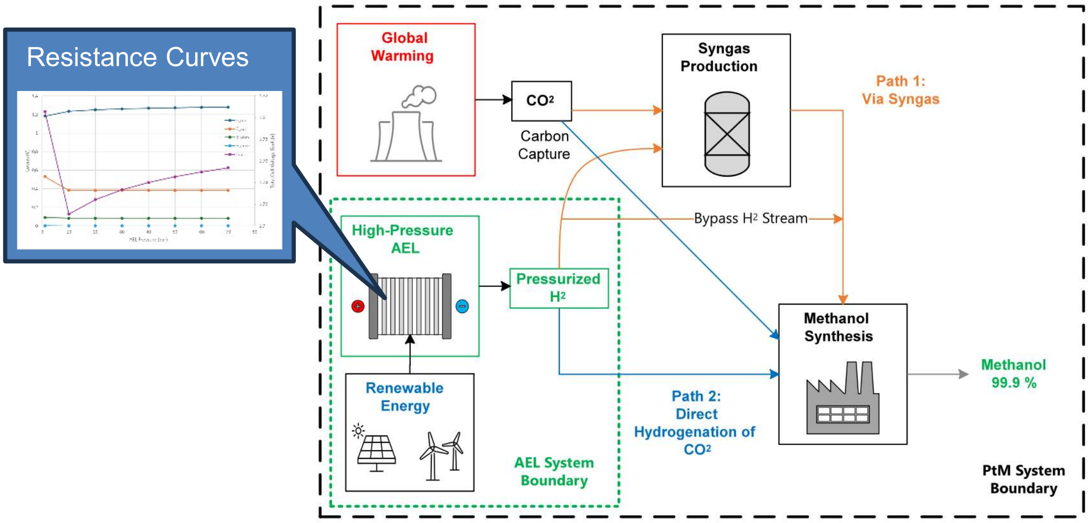

Figure 1: Block flow diagram for power-to-methanol (PtM) process via two pathways.

Results

The optimal AEL configuration achieved the lowest NPC of H_2 at moderate pressure is consistent with the expected decrease in ohmic resistance and improved ionic conductivity. However, this case was not optimal at the PtM system level, where matching electrolyzer pressure with methanol reactor and recycle pressures shifts the cost balance toward reduced compression demand. The results demonstrate that optimizing the AEL unit in isolation does not ensure overall process efficiency, as PtM system-level interactions in particular pressure and thermal coupling with the downstream methanol synthesis play a decisive role in determining total performance. The lowest methanol NPC was achieved when AEL pressure and reactor pressure were integrated. At higher AEL pressures, Faraday efficiency decreased due to increased dissolved gas crossover and recombination losses, increasing hydrogen production cost and total cell voltage, confirming trends observed in Abdin et al.[3] and Sánchez Delgado[4].

Conclusions

High-pressure AEL improves downstream compatibility but becomes counter-productive at very high pressures due to crossover-driven efficiency losses and internal resistances. Economically, the analysis highlights that reducing electricity costs through improved integration and flexible operation offers the greatest leverage for lowering the net production cost of methanol. The automated Aspen-Python workflow developed at DLR enables rapid multi-parameter techno-economic analysis (TEA).

Characterisation of Bubble Size Distribution in a Vertical Water Electrolyser

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Hydrogen produced via water electrolysis (WE) plays a key role in achieving net-zero carbon dioxide emissions and is a sustainable storage solution for addressing the intermittency of renewable energy sources [1]. Among available WE technologies, Alkaline stands out for its maturity and scalability [1]. However, improving its low efficiency remains a challenging task. Gas products cause a significant energy loss. Efficient bubble detachment from the electrode surface reduces transport overpotentials and, consequently, energy consumption [1]. Thus, investigating bubble size distribution is quite important as it directly influences key two-phase flow parameters. Bubble diameter is affected by factors such as electrode geometry, current density, and flow regime. In this work, the evolution of gas bubbles in a vertical alkaline water electrolyser is experimentally investigated. Bubble formation, growth, and detachment are visualised using a high-speed camera under controlled current densities and Reynolds numbers. The recorded images, Figure 1(a), are analysed in MATLAB using image-processing functions to extract information on bubble size distribution, Figure 1(b). Oxygen bubbles form at the anode on the right-hand side, while hydrogen bubbles form at the cathode on the left-hand side. The bubble size distributions will be used as input for two-phase flow Computational Fluid Dynamics (CFD) simulations to gain insights into the gas-liquid interactions in water electrolysis systems.

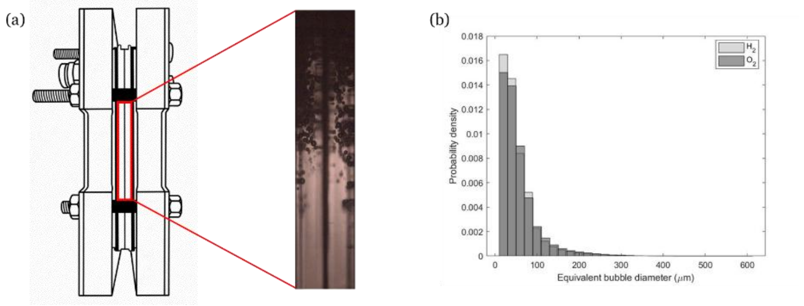

Figure 1. (a) Schematic view of the vertical electrolyser and visualisation window showing gas bubble formation captured by a high-speed camera. (b) Bubble size distribution histogram for H_2 and 0_2 bubbles at $\mathrm{Re} = 25$ and $I = 400\ \mathrm{mA\ cm^{-2}}$.

Acknowledgements:
This work was supported by: (i) ATE - Alliance for Energy Transition (56) co-funded by the Recovery and Resilience Plan (PRR) through the European Union, and (ii) Fundação para a Ciência e a Tecnologia, I.P./MECI through national funds: LSRE-LCM, UID/50020/2025 (https://doi.org/10.54499/UID/50020/2025); and ALiCE, LA/P/0045/2020 (https://doi.org/10.54499/LA/P/0045/2020). Margarida L.R. Peixoto acknowledges FCT for the financial support with reference 2024.00676.BD.

References:
1. Liu, Y., S. Li, H. Wu, and Y. Shi, *Experimental investigation and analysis for the bubble size distribution during alkaline water electrolysis by using a wire electrode.* DeCarbon, 2024. **5**: p. 100052.

Keywords: Water electrolysis, Green Hydrogen, Gas Bubbles, Vertical Electrolyser.

Dynamic System Modeling of Alkaline Water Electrolysis Including Natural Convection and Degradation Effects

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Abstract

Alkaline water electrolysis (AWE) is a mature and robust technology for large-scale hydrogen production, yet its dynamic behavior under realistic operating conditions remains insufficiently represented in system-level models. In this work, a physics-based system model for alkaline water electrolysis is developed with the aim of capturing the coupled electrochemical, thermal, and fluid-dynamic behavior of an AWE system while maintaining computational efficiency.

The model describes the electrochemical performance of the electrolyzer stack based on fundamental voltage contributions and is embedded into a system framework including thermal management and electrolyte circulation. Experimental data obtained from a laboratory-scale AWE test bench is used for model calibration and validation, demonstrating good agreement in terms of cell voltage, temperature evolution, and system response under varying operating conditions.

To extend the applicability of the model, an approach for incorporating natural convection effects within the electrolyte is proposed. This enables a more realistic representation of heat and mass transport, particularly under low flowrate and part-load operation. Furthermore, a modeling strategy for the inclusion of degradation effects is presented, allowing long-term performance changes to be assessed based on operating history.

The developed system model provides a versatile tool for the analysis, optimization, and design of alkaline water electrolysis systems and supports the evaluation of operational strategies with respect to efficiency, thermal behavior, and lifetime.

Keywords: ModVal2026, alkaline electrolysis, system model, natural convection, degradation

Using physics-based models as data-driven ones: a new approach for modelling fuel cells and electrolyzers

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Abstract

Fuel cell and electrolyzer models are typically categorized as either physics-based or data-driven, with some hybrid approaches combining elements of both. Physics-based models offer interpretability and access to internal variables representing the underlying phenomena, and they can often be calibrated using a limited amount of experimental data. Data-driven models, in contrast, typically require large datasets for training, since the input-output relationship is learned directly from data and must be assessed using procedures such as cross-validation to limit overfitting and quantify generalization. For physics-based models, using similarly large datasets is often not feasible because commonly used 1D or higher-dimensional models are computationally demanding. The long computational times involved limit large-scale parameter estimation, extensive sensitivity analyses, and evaluation across many operating conditions.

We propose a novel approach that leverages ultra-fast 0D physics-based models as if they were data-driven ones. By using a steady-state 0D formulation with explicit equations, we avoid iterative nonlinear solvers. This makes simulations fast enough for large-scale calibration and cross-validation on a sizeable dataset, even with many parameters to estimate. Inspired by data-driven methodologies, our workflow uses a large set of polarization curves and high-frequency resistance (HFR) measurements under varying operating conditions to build robust models with strong predictive capability. We demonstrate this approach for low-temperature proton exchange membrane (PEM) fuel cells, achieving a root mean square error (RMSE) below 20 mV for operating conditions not included in the training dataset (eight operating conditions used for training). Unlike purely data-driven models, the 0D physics-based model also provides access to internal variables such as catalyst-layer temperature, membrane water content, and liquid water saturation in porous layers, enabling physical interpretation and providing a consistent basis for future integration of degradation models.

Currently, we are extending this methodology to PEM fuel cells in diverse applications, including maritime, heavy-duty mobility, and unmanned aerial vehicles (UAV), as well as to anion exchange membrane water electrolysis (AEMWE). Our long-term goal is to adapt this framework to a broader range of electrochemical systems, further advancing the robustness and applicability of 0D physics-based modeling.

Keywords: 0D models, physics-based models, fuel cells, electrolysers, parameter estimation

Poster Abstracts

Session B: Energy Conversion

Session B6: CO_2 electrolysis

Model-Based Optimization of Cathode Architecture and Bipolar Membrane Properties in Bicarbonate-Fed CO_2 Electrolyzers

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Bicarbonate-fed bipolar membrane (BPM) electrolyzers offer a compelling pathway for carbon monoxide (CO) production by directly valorizing captured carbon without the need for energy-intensive CO_2 regeneration and compression. However, their performance is strongly constrained by coupled transport, reaction, and membrane phenomena that govern local pH, CO_2 availability, hydrogen evolution, and cell voltage. A systematic, physics-based understanding of how cathode architecture, operating conditions, and BPM properties interact is therefore essential for rational device optimization.

In this work, we develop a one-dimensional, volume-averaged numerical model of a bicarbonate-fed BPM CO_2-to-CO electrolyzer, resolving water dissociation in the BPM, ionic transport, bicarbonate-to-CO_2 regeneration, gas–liquid mass transport, and electrochemical reaction kinetics within the porous cathode. Using this framework, we first investigate the impact of cathode design parameters—including catalyst layer (CL) mass loading, CL porosity, porous carbon substrate porosity, and substrate thickness—on local reaction environments, CO faradaic efficiency, and cell voltage. In parallel, we quantify the influence of operating conditions such as bicarbonate concentration, inlet electrolyte pH, and total inlet gas pressure on CO_2 availability, proton utilization, and selectivity toward CO versus hydrogen evolution.

The model reveals strong trade-offs between CO_2 transport, local alkalinity, and electronic and ionic resistances, leading to well-defined optimal ranges of CL structure and substrate properties that maximize CO selectivity while limiting voltage losses. Higher bicarbonate concentrations and controlled inlet pH are shown to enhance CO_2 regeneration and utilization, whereas elevated inlet gas pressures improve CO_2 solubility but impose additional transport constraints. Building on the optimized cathode architecture and operating conditions, we subsequently investigate BPM optimization strategies in which membrane hydration, ion-exchange capacity, and thickness are varied independently for the cation- and anion-exchange layers. This asymmetric membrane design space is systematically explored to exploit BPM asymmetry and optimize the current density sustained through the BPM. The results demonstrate that targeted BPM optimization can simultaneously reduce the required cell voltage and further suppress parasitic hydrogen evolution without compromising CO production. Model predictions are consistent with in-house experimental trends, highlighting the combined importance of cathode and BPM co-design. Overall, this work provides a quantitative modeling framework and clear design guidelines for improving selectivity and energy efficiency in bicarbonate-fed BPM electrolyzers, supporting the development of scalable carbon utilization technologies.

Keywords
Bicarbonate electrolysis, bipolar membrane, cathode optimization, CO_2-to-CO modeling

Studying Local Inhomogeneities in Zero-gap CO_2 Electrolysis via Validated 2D Multiphysics Simulation

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Abstract

Zero-gap membrane electrode assemblies (MEAs) are critical for industrializing electrochemical CO_2 reduction (CO_2R), yet scale-up is hindered by localized current density fluctuations and species crossover, affecting selectivity and single-pass conversion. Physics-based modeling provides a better understanding of performance degradation by identifying how it is driven by coupled along-the-channel gradients and water-management issues. This work reports a two-dimensional (2D), continuum-scale, steady-state model to spatially resolve and study the transport in porous media and electrochemically induced effects within a CO_2-to-CO electrolyzer. The domains cover the entire zero-gap MEA: a flow-through gas diffusion layer (GDL) coated with Ag catalyst, an anion-exchange membrane (AEM), and a porous anode adjacent to a flow channel fed with anolyte.

Validation is performed via a 32-segmented current collector cell, providing experimental resolution of the local current density along the flow. The model explicitly accounts for liquid water transport (including electro-osmotic drag) and quantifies the influence of saturation and salting-out on cathode catalyst accessibility, emphasizing the role of water management. This 2D approach captures the complex interplay between through-plane transport and along-the-channel changes in species' concentration and selectivity, also clarifying the impact of feed pressure and relative humidity. Furthermore, resolving the anodic compartment reveals how gaseous CO_2 regeneration competes with O_2 evolution and dictates the tertiary current distribution. Results demonstrate that 2D refinement is essential to explain the spatial depletion and selectivity shifts observed experimentally. This study thus identifies origins of mass-transport limitations in zero-gap cells, providing a quantitative basis for the design and further scale-up of CO_2 electrolysis stacks.

Acknowledgements: This work is funded by the Swiss State Secretariat for Education, Research and Innovation (SERI) and is part of the European Commission's Marie Skłodowska-Curie doctoral network MiEl. Under the HORIZON programme, the MiEl project received funding by the European Union via the Grant Agreement No. 101073003.

Keywords: ModVal2026, CO_2 electrolysis, zero-gap MEA, multiphysics modeling, species crossover

Hydrogen production by combined hydrothermal liquefaction and membraneless electrochemical reforming of organic waste with integrated CO_2 capture

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Abstract

Electrochemical reforming is a promising process to produce hydrogen from the reduction of water while oxidizing an organic waste compound [1]. Researchers are commonly not considering that the most common organic waste substrates are a variety of more complex polymeric chains. The integration with electrolysis of their depolymerization to simpler molecules has not been fully explored yet. The process produces CO_2, which needs to be captured and sequestrated to minimize its environmental impact.

We propose a novel process that integrates the hydrolysis of organic waste via hydrothermal liquefaction (HTL) and CO_2 capture via salt precipitation into electrochemical reforming. We developed a physics-based model to describe the HTL of four organic waste feedstocks (wood, algae, municipal sludge and agricultural waste) to simpler organic molecules and their complete oxidation at the anode of a membraneless electrolyzer while producing hydrogen at its cathode [2]. The separation of products is obtained imposing a convective flux of liquid electrolyte without a solid separator, the electrolyzer may therefore operate at the same temperature as the HTL (250 °C < T < 350 °C). The CO_2 produced in the process is captured as carbonate anions (CO_3^{2-}), its most stable thermodynamic form in strongly alkaline conditions (pH > 12.5) [3]. The carbonate ions in solution may be sequestrated as solid carbonate salt (Na_2CO_3) by cooling down the solution and separating the liquid phase. The integrated three-step process ensures a combined waste treatment and full-chain CO_2 capture and sequestration. Thermal integration and the use of the strong base for multiple purposes (catalyst for hydrolysis, charge carrier for electrolysis and sorbent for CO_2 capture) ensures a better efficiency than the three individual processes.

We predict the optimal operating conditions for the combined HTL and electrolysis are in the range 308 °C – 312 °C with a biomass to solvent ratio between 6.0 % and 7.7 % for the four feedstocks. Operation at this temperature decreased the kinetic and ohmic overpotentials, respectively, by approximately 35 % and 73 % with respect to 50 °C. Agricultural waste is the most suitable substrate due to its maximal integrated efficiency of η_{HTL+EC} = 44%. Its large fraction of lipids (which have the highest bio-oil yield during HTL) was the main parameter affecting the efficiency at the same operating conditions.

The first validation of the innovative configuration of the membraneless electrolyzer was performed oxidizing ethylene glycol and glycerol at 60 °C. A current density of 50 mA cm^{-2} was achieved applying a voltage of 1.2 V. CO_2 capture as carbonate anion was confirmed by ^{13}C NMR. The sequestration of the carbonate salt was instead performed without any energy input using a calcium precursor. A sequestration efficiency above 99% was achieved at least 1000x faster than geological sequestration.

The process proposed defines a new approach towards the production of *circular* green hydrogen from organic waste partially capturing CO_2, a combination of different features which are fundamental to reach the target of a net-zero emitting society by 2050.

Keywords: Membraneless – Electrochemical Reforming – Hydrogen – CO_2 Capture

References

[1] C. Lamy, C. Coutanceau, S. Baranton, *Production of Clean Hydrogen by Electrochemical Reforming of Oxygenated Organic Compounds*, Academic Press, **2019**.
[2] R. Valenza, M. Bruno, S. Haussener, “Integrated hydrothermal liquefaction and membraneless electrolysis of organic waste for hydrogen production and CO2 capture” *Prep.* **n.d.**
[3] Z. Rastegar, A. Ghaemi, “CO2 absorption into potassium hydroxide aqueous solution: experimental and modeling” *Heat Mass Transf.* **2022**, *58*, 365–381.

Using simulations and machine learning for efficient electrochemical CO2 reduction for ethylene production

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Abstract

Low-temperature CO_2 electrolysis for ethylene production presents significant potential to reduce fossil fuel reliance within the chemical industry. Although there have been notable recent advancements, the process's key performance indicators (activity, selectivity, and durability) remain inadequate for large-scale industrial adoption. In this study, data derived from multi-physics simulations are utilized to develop a surrogate machine learning model, which is then employed to optimize the membrane-electrode-assembly configuration of a zero-gap cell.

A one-dimensional continuum model was developed to simulate the coupled processes concerning gas and liquid flow, species transport, and heterogeneous and homogeneous reactions. The model is validated against the existing literature experimental and modelling data. Subsequently, for a defined set of kinetics, the model was employed to systematically examine a wide range of cell configurations, with particular emphasis on variations in cathode and membrane properties. The effects of these parameters on the I-V characteristics, Faradaic efficiency, and spatial distributions of key concentrations will be presented.
Later, machine learning methods are applied on the dataset to (i) determine the key cell parameters as a function of the applied voltage and (ii) develop an accelerated surrogate model for use within an optimization algorithm. While linear models do not reliably predict simulated cell performance, both random forest regressors and neural networks yield accuracies with less than 10% relative error. Finally, a machine learning-based optimization is conducted to concurrently maximize power density and partial current density.

Keywords: CO_2 Electrolysis, Ethylene Production, Multiphysics, Surrogate Modeling, Machine Learning Optimization

Investigating Morphological Evolution and Degradation of Electrocatalysts During Electrochemical CO_2 Reduction

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Abstract

Electrochemical CO_2 reduction in gas diffusion electrodes in flow-cell configurations offers a promising route for sustainable fuel production, yet long-term catalyst stability remains a key limitation. Under realistic operating conditions, morphological restructuring of electrocatalyst layers, as well as electrolyte flooding and salt precipitation, strongly impact performance. A systematic pore-scale analysis of such dynamic changes is thus essential for guiding the rational design of stable and efficient CO_2 reduction catalysts.

We develop a combined imaging and modelling framework to investigate the temporal evolution of electrocatalyst morphology during CO_2 reduction. High-resolution FIB-SEM nano-tomography is used to generate 3D reconstructions of Ag catalyst layers. Initial work focuses on the pristine state of the sample, providing a detailed digital reconstruction for structural and transport analyses. Complementary SEM and EDX characterization are used to assess morphological and compositional changes before and after electrochemical operation, providing guidance for selecting critical time points for subsequent 3D reconstructions to capture key stages of catalyst degradation. This then enables ex-situ tracking of morphological alterations over time. These reconstructed digital catalyst architectures are analysed within a pore-scale modelling framework to quantify the evolution of key structural and effective transport properties, including surface area, porosity, tortuosity, and effective transport coefficients.

This approach aims to enhance the understanding of the dynamic behaviour of electrocatalysts during CO_2 reduction, initially focusing on gaining insight into morphological changes and their influence on the device's performance.

Keywords: ModVal2026, Electrochemical CO_2 reduction, Catalyst Degradation, Gas Diffusion Electrode, FIB-SEM nano-tomography, Pore-Scale Modelling

(Micro-)kinetic Effect on Selectivity during Pulsed Electrolysis: Exploring the Space of Electrochemical Parameters

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Abstract

Electrolysis is usually performed under constant potential or current, but pulsed electrolysis has received growing attention over the last years, especially in the context of CO_2 reduction where favorable impacts on product selectivity are observed. However, the mechanism at play remains under debate.[1,2] The role of (micro-)kinetics events during transient operation has received little attention compared to other effects such as mass-transport or surface modification. Herein, we model electrochemical reactions following classical theory of electron transfer and chemical reaction rate. Upon conditions where mass-transport effect and surface modification are not interfering, we show that some cases are subjects to strong selectivity improvements (exceeding 5000% for some cases), resulting only from (micro-)kinetics effects. We derive a method for pulsed program optimization and explore the space of electrochemical parameter with Monte-Carlo simulation. This study provides a way to predict experimental cases for which the (micro-)kinetic phenomena are likely to dominate the selectivity response under pulsing. It also shows that some high selectivity improvements are compatible with high current density operation, relevant for commercially-viable CO_2 reduction.

References

(1) Casebolt, R.; Levine, K.; Suntivich, J.; Hanrath, T. Pulse Check: Potential Opportunities in Pulsed Electrochemical CO2 Reduction. Joule 2021, 5 (8), 1987–2026.
(2) Miličić, T.; Sivasankaran, M.; Blümner, C.; Sorrentino, A.; Vidaković-Koch, T. Pulsed Electrolysis – Explained. Faraday Discuss. 2023, 246 (0), 179–197.

Keywords: ModVal2026, Pulse electrolysis, Microkinetic, Selectivity, Monte Carlo

The Cathode Ionomer as an Interfacial Modulator in Electrolyte-Free CO_2 Electrolysis

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Abstract

Gas-fed, zero-gap CO_2 electrolyzers commonly rely on alkali metal cations to enhance activity and selectivity by structuring the electric double layer (EDL) and stabilizing key reaction intermediates. However, delivering these cations via liquid electrolytes introduces challenges such as uncontrolled ion crossover, salt precipitation, and flooding, which compromise durability. Here, we investigate whether fixed-charge ionomers in the cathode catalyst layer can reproduce the beneficial effects of free cations in an electrolyte-free configuration.

Using a fully gas-fed membrane electrode assembly in which the ionic environment is strictly controlled, we show that even trace amounts of residual alkali cations introduced during membrane pretreatment measurably influence CO_2 reduction performance, confirming their accumulation at the cathode and their role in shaping the EDL. Beyond these mobile cations, we demonstrate that the ionomer itself plays a decisive electrochemical role. Systematic variation of the ionomer ion-exchange capacity (IEC) reveals that high-IEC ionomers significantly reduce cathode overpotential, enhance interfacial pseudocapacitance by more than an order of magnitude, and markedly improve short-term stability under pure-gas operation. These effects are attributed to the ability of fixed organic cations to modulate the interfacial electric field, local hydration, and charge storage in the absence of continuous cation supply.

Together, our results establish catalyst-layer ionomer design as a powerful lever for controlling interfacial chemistry in electrolyte-free CO_2 electrolysis and provide a framework for developing durable, simplified zero-gap devices that do not rely on liquid electrolytes.

Keywords: CO_2 electrolysis, Pure-water operation, zero-gap, electrical double layer, ionomer, catalyst layer

Poster Abstracts

Session B: Energy Conversion

Session B7: Transport in electrodes and membranes, and diagnostics

Insight on in-cell three-electrode EIS using an insulated endplate as pseudo-reference

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Abstract

A three electrode EIS allows to analyze the behavior of cathode and anode separately, disentangling the electrode activation energies from the membrane resistance. However, a three-electrode analysis is often difficult to be performed in an in-cell fully operational context due to the lack of space for a reference electrode and the need to keep the cell sealed and compressed. The use of dedicated cells with microelectrodes or ex situ three electrode setups usually forces a design not representative of the real condition with large separation between the electrodes and consequently a high resistance and limitation for the current density.
Here we propose an alternative method to achieve a three electrode EIS for anode and cathode separately in an operating representative test monocell by using the existing cell endplate (316L stainless steel) electrically insulated from the two electrodes as a pseudo-reference electrode for the measurement of anodic and cathodic potential. Our method does not require any special hardware and can be applied on the existing design representative of the real stack operative condition, without affecting the measurement of the high frequency cell resistance. Drifts of the potential of the pseudo-reference electrode, e.g. due to variations of ion and oxygen concentration in the electrolyte and oxidation status of the material, normally happen with time scales so long that they do not affect the EIS high frequency measurements, so that the pseudo-reference may be considered as stable as standard Hg/HgO or Ag/AgCl reference electrodes, but with the advantage that it does not require extra space nor cell modifications for its installation.

The results for separate anode and cathode spectroscopy loops, collected simultaneously on two different channels, are discussed in wet and dry cathode configuration. A particular insight is given to the low frequency inductive loop appearing in the dry cathode configuration yielding indirect information on the wetness status of the dry cathode. Moreover, the ohmic component of the short and bubble free electrolyte gap between working and reference electrode not including the membrane gives an online measurement of the electrolyte conductivity with no need of a dedicated probe.

Keywords: ModVal2026, EIS, pseudo-reference electrode, low frequency inductance

Definition and Interpretation of Concentration and Activation Overpotentials

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Abstract

For electrochemical systems, the cell potential is frequently divided into separate overpotential contributions to quantify the energetic losses associated with different physical phenomena [1,2]. Among the key overpotentials are the activation overpotential $\boldsymbol{\eta}_{\mathrm{act}}$ due to limited reaction kinetics and the concentration overpotential $\boldsymbol{\eta}_{\mathrm{conc}}$ due to limited mass transfer. However, these overpotentials are not always defined consistently. For example, the concentration overpotential $\boldsymbol{\eta}_{\mathrm{conc}}$ is most commonly defined as the shift in equilibrium potential due to limited mass transfer [3,4,5]. Even though it has been pointed out that this definition does not describe the effect of mass transfer on the cell potential at large $\boldsymbol{\eta}_{\mathrm{act}}$ [5,6], it is frequently applied also in that case. While an alternative definition of $\boldsymbol{\eta}_{\mathrm{conc}}$ exists to describe the effect of mass transfer on the cell potential at any $\boldsymbol{\eta}_{\mathrm{act}}$ [6], it appears less frequently applied and only together with the Tafel approximation for high $\boldsymbol{\eta}_{\mathrm{act}}$. Overall, a discussion of the varying definitions and their implications appears to be missing.

To this end, we discuss the definitions and interpretation of $\boldsymbol{\eta}_{\mathrm{act}}$ and $\boldsymbol{\eta}_{\mathrm{conc}}$ [7]. We show that the different definitions of $\boldsymbol{\eta}_{\mathrm{act}}$ and $\boldsymbol{\eta}_{\mathrm{conc}}$ i) cannot be chosen independently when dividing the cell potential into additive contributions, ii) can lead to largely different overpotential values, and iii) associate a different meaning with each overpotential. Especially the often-considered definition of $\boldsymbol{\eta}_{\mathrm{conc}}$ as the shift in equilibrium potential due to limited mass transfer can lead to misleading results. To demonstrate the practical relevance, we apply the definitions to assess the effect of gas supersaturation on the cell potential during water electrolysis: Under typical operating conditions, the effect on the cell potential is shown to be likely much smaller than what is suggested in literature works that define $\boldsymbol{\eta}_{\mathrm{conc}}$ as the shift in equilibrium potential.

References:

[1] Haverkort & Rajaei (2021). J. Power Sources, 497, 229864.
[2] Hammoudi, et int., Doumbia (2012). Int. J. Hydrogen Energy, 37(19), 13895–13913.
[3] Zhao, Ren, Luo (2019). Langmuir, 35(16), 5392–5408.
[4] Leistra & Sides (1987). J. Electrochem. Soc., 134(10), 2442–2446.
[5] Hamann, Hamnett, Vielstich (2007). Electrochemistry: Wiley-VCH.
[6] Enyo & Yokoyama (1970). Electrochim. Acta, 15, 183–191.
[7] Seidenberg, Mitsos, Bongartz (2025). J. Electrochem. Soc., 172(4), 043506.

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Keywords: ModVal2026, electrolysis, overpotentials, mass transfer

Modeling of electrochemical impedance spectroscopy measurements under gas evolution

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Abstract

The underlying causes of efficiency losses in electrochemical cells are often assessed using the impedance obtained from electrochemical impedance spectroscopy measurements. The impedance of gas evolution reactions, e.g., the oxygen evolution reaction, has been modeled with electric circuits representing electric resistance, reaction kinetic, and mass transfer effects [1-3]. However, such electric circuits have not been derived specifically for gas evolution reactions. Therefore, it is not self-evident that they sufficiently capture relevant gas bubble effects.

To clarify this aspect, we derived an expression for the impedance of a gas evolving system starting from a time-domain model. In contrast to literature, the impedance expression includes a second electric resistance contribution (in addition to the often-considered, static electric resistance) as well as an electrode coverage contribution. Particularly the second electric resistance contribution is expected to be considerable under significant gas evolution. It is a result of the current density dependency of the electric resistance due to gas bubbles. Thus, it is linked to the gas bubble dynamics and therefore frequency dependent. We apply the derived impedance expression to evaluate impedance data obtained for the alkaline oxygen evolution reaction in a three-electrode beaker cell setup [4] under industrial conditions. Using this data, we demonstrate the presence of the second electric resistance contribution in the low-frequency range and show that it has a considerable magnitude for current densities larger than 500 mA/cm^2. Overall, the developed impedance expression can help to correctly identify different loss mechanisms based on EIS data.

References:

[1] Ikeda, et int., Misushima. (2022). Electrochim. Acta, 430, 141053.
[2] Chmielowiec, et int., Allanore (2019). J. Electrochem. Soc., 166(10), E323-E329.
[3] Wang, et int., Thorpe. (2025). Electrochim. Acta, 518, 145784.
[4] Thissen, et int., Mechler. (2024). ChemElectroChem, 11(1), e202300432.

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Keywords: ModVal2026, electrolysis, hydrogen, gas bubbles, EIS

Coupled electrochemical–MHD modeling of magnetic-field-induced water electrolysis in acidic electrolyte

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Abstract

The UK aims to deploy 10 GW of low-carbon hydrogen production capacity by 2030, yet the choice of dominant production technology remains under discussion. At present, around 95% of global hydrogen is produced via steam methane reforming, which generates substantial CO_2 emissions and therefore relies on extensive carbon capture to approach carbon neutrality. Renewable-powered water electrolysis offers a route to truly green hydrogen, but it is not yet cost-competitive due to high capital (CAPEX) and operating (OPEX) costs. Advancing current electrolyzer technologies, and exploring new approaches, is therefore essential. Given the UK's strong offshore wind resource, this work investigates a concept that uses wind-turbine mechanical power directly, combined with magnetic-field-influenced electrolysis, for hydrogen production. We consolidate and connect the relevant physics governing the electrolysis, including electrochemistry, electromagnetism, turbulent fluid flow, ionic species transport (diffusion, migration, and convection), and magnetohydrodynamic (MHD) effects. Multiphysics modeling in COMSOL will be used to develop a digital twin of the system, enabling interpretation of coupled phenomena and guiding optimization.

Keywords: Green hydrogen; Offshore wind; Multi-physics; Electrochemistry; Electromagnetics; Magnetohydrodynamics

Local Lattice Boltzmann Implementation for Electrochemical Transport in OpenLB

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Abstract

Simulating electrochemical phenomena in porous electrodes at the pore scale combines the challenges of complex multiphysics couplings and complex 3D geometries. The Lattice Boltzmann Method (LBM) offers an attractive alternative for this class of problems due to its ability to easily handle complex 3D domains, ease of implementing local couplings, and inherent parallel efficiency. However, implementations for specific features of electrochemical processes—such as Butler-Volmer kinetics, charge transport under electroneutrality constraints, or Nernst-Planck ion transport—are not readily available in open-source libraries.

In this work, we present an implementation of the relevant physics within the framework of OpenLB, an open-source LBM library. The implementation solves coupled fluid flow, advection-diffusion-migration, charge conservation, and electrochemical surface reactions via fully local couplings to take advantage of OpenLB's parallelization capabilities. The code is validated against benchmark problems proposed by He and Li, namely convective diffusion, ion migration, and a general case incorporating diffusion, convection, and migration. Our code successfully reproduces the analytical benchmarks, enabling large-scale simulations of electrochemical systems using LBM.

Keywords: Lattice Boltzmann Method, Nernst-Planck, Electrochemical Systems, OpenLB

Energy and Exergy Balancing in Modular Electrochemical and Fluid Dynamic Systems Modelling

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Abstract

System modelling is a helpful tool in the early stages of process development. In order to analyze different system scenarios regarding their thermodynamic efficiency we implemented an automatic energy and exergy calculation in our modelling that allows the analyzation of the influences of design and process parameters as well as application scenarios and different system architectures. The modelling focused on electrochemical and fluid dynamic systems is done in the language modelica, that is an object-oriented approach in which components inherit properties from more general hierarchical component definitions. This enables the modelling of reusable, extensible models where specialized components automatically obtain equations, parameters and interfaces defined at higher levels in the model structure.

For the automized energy and exergy balancing we implemented a base class called component wrapper that can be used to model components and contains the relevant interfaces as well as the energy and exergy calculations. The principle of the component wrapper is shown in Figure 1 on the left. This base class defines fluid, heat, power and electrical inputs and outputs of the component, that can be used depending on the kind of component. Defined by the enthalpy in- and outflow (H_{in} and H_{out}) of one component the heat, power and electrical demand can be determined and the balancing can be done. In the case of chemical reactions, the reaction enthalpy is evaluated as well.

By using the component wrapper to model each component the balancing is possible on component as well as on system level by interconnecting single components and can be visualized with Sankey-diagrams for energy flows as shown in Figure 1 on the right and Grassmann-diagrams for exergy flows. This work aims to enable a scientifically sound and fair energetic evaluation of energy systems. With the exergy balancing the possibility of the thermodynamic optimization via the evaluation of usability of the energy and therefore the optimization of system architectures is created. This methodology will be presented on examples of different electrochemical system designs focused on hydrogen applications.

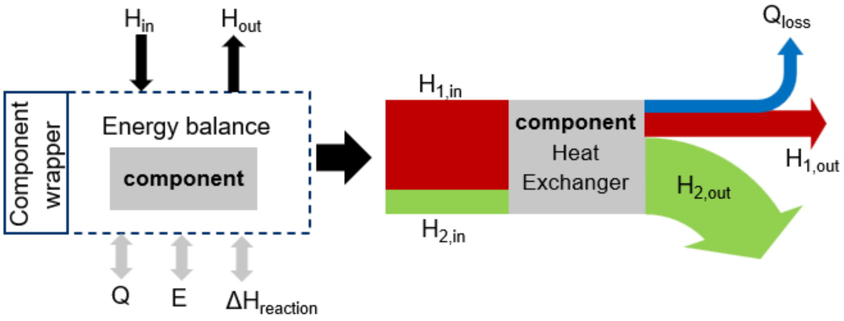

Figure 1: Principle of Energy balancing and Sankey Diagram example for heat exchanger

Keywords: ModVal2026, electrochemical system modelling, Energy balancing, Thermodynamic optimization

Modeling and simulation of a closed electrochemical cell via an ion-conserving modified Poisson–Boltzmann model with dielectric decrement

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Abstract

We present a mathematical and numerical model of a closed nanoscale electrochemical cell in equilibrium, which takes into account finite ion sizes, momentum balance, and dielectric permittivity that depends on field strength and ion concentrations. To consider the closed character of the cell, the model is amended using an integral constraint on the number of ions within the system. We present the first set of simulation results, which examine the influence of dielectric decrement and overlapping double layers on ionic concentration, potential distributions, and the resulting capacitance curves. The model was developed during the IPAM Long Program titled "Bridging the Gap: Transitioning from Deterministic to Stochastic Interaction Modeling in Electrochemistry" with the aim to compare continuum and molecular dynamics simulations. Variants of the model have been implemented in MATLAB® and the Julia package AugmentedPoissonBoltzmann.jl.

[1] Dreyer, W., Guhlke, C., & Landstorfer, M. (2014). A mixture theory of electrolytes containing solvation effects. Electrochemistry communications, 43, 75-78.

[2] Landstorfer M, Müller R (2022) Thermodynamic models for a concentration and electric field dependent susceptibility in liquid electrolytes. Electrochim Acta 428:140368

[3] Sugioka, H. (2016). Ion-Conserving Modified Poisson–Boltzmann Theory Considering a Steric Effect in an Electrolyte. Journal of the Physical Society of Japan, 85(12), 124006.

[4] J. Fuhrmann, M. Landstorfer, J. Landini, K Thornton. AugmentedPoissonBoltzmann.jl - Poisson-Boltzmann solver with finite ion sizes, solvation, dielectric decrement and ion conservation. https://github.com/IPAM-ECH2025/AugmentedPoissonBoltzmann.jl

Keywords: Poisson-Boltzmann, Steric Effects, Dieelectric Decrement

Poster Abstracts

Session B: Energy Conversion

Session B8: Solar-driven electrochemsitry

Investigation of a tandem membrane-photoelectrode assembly for solar hydrogen production

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Abstract

Photoelectrochemical (PEC) water splitting is a promising approach for the direct conversion of solar energy to renewable hydrogen. Tandem photoelectrode systems with a coupled photocathode and photoanode materials have been proposed to maximize the harvesting and conversion of photons to chemical products. However, the integration of these tandem PEC reactor designs with proton exchange membranes (PEMs) remains largely unexplored. Here, we demonstrate the first tandem PEC–PEM water splitting cell operating with pure milli-Q water in liquid phase. The device employs semiconductors deposited on a transparent, porous, conductive substrate (TPCS) [1], functionalized with ionomers, that enables both electron conduction from the photoelectrodes to an external circuit and ion transport through the photoelectrodes and across the membrane. A wider-band-gap semiconductor ($BiVO_4$) was used as the photoanode, while a lower-band-gap organic semiconductor (PBDB-T:ITIC) served as the photocathode, allowing enhanced utilization of the solar spectrum. The system achieved unbiased water splitting for hydrogen production under 1 sun illumination (100 mW cm^{-2}), demonstrating the feasibility of fully green hydrogen generation without any external power supply. A current density of 0.009 mA cm^{-2} was obtained at zero applied cell voltage, corresponding to a solar-to-hydrogen (STH) efficiency of 0.011%. Additional measurements under increased irradiances (up to 32 suns) revealed an enhanced photocurrent density. The unbiased photocurrent generation increased 5-fold to 0.05 mA cm^{-2} under 6 suns. However, at higher irradiances (> 6 suns) a photocurrent saturation was observed yielding marginal benefits. Despite the relatively low performance in terms of STH efficiencies compared to the more traditional approach of using planar electrodes and supporting electrolytes, this work establishes a novel tandem PEC–PEM reactor design using milli-Q water and outlines key pathways for future improvements toward efficient solar-driven hydrogen production.

Keywords: ModVal2026, Photoelectrochemical (PEC) reactor, Tandem cell, PEM

[1] Caretti, Marina, Elizaveta Mensi, Raluca-Ana Kessler, et al. “Transparent Porous Conductive Substrates for Gas-Phase Photoelectrochemical Hydrogen Production.” Advanced Materials 35, no. 9 (2023): 2208740.

Current decay curves and degradation of oxynitride photoanodes for renewable hydrogen generation

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Abstract

Because of its comparatively simple design photoelectrochemical (PEC) water splitting shows promise as a cost-effective technology for future green hydrogen production [1,2]. While the efficiency of PEC systems has been significantly improved over the last decades, their stability remains a major challenge [2]. Based on several technoeconomic studies, operation for at least two years without significant performance loss is required for an economically viable implementation of PEC devices [1, 3]. Since most PEC electrodes degrade on a time scale of hours instead of years, stability improvements of PEC systems are mandatory. Investigating the degradation processes of photoelectrodes is therefore important from both scientific and practical perspectives, as it is crucial for developing photoelectrodes with longer lifespans. Since oxynitrides are known for their excellent performance with respect to efficiency for water oxidation [4], the current decay curves of oxynitride-based photoanodes were studied.

In this contribution, we compare the current decay curves of oxynitride electrodes by acquiring chronoamperometries at 1.23 V vs RHE. Guided by the excellent correlation between the measured chronoamperometries and the curves obtained by fitting with the sum of two exponential decay functions, we identified two current decay processes. We propose that the process occurring on shorter time scales was of capacitive origin, while the decay process with the longer time constant was attributed to degradation. This time constant was suggested as an alternative figure of merit for quantifying the stability of oxynitride based photoanodes. The applicability of this figure of merit to a wider range of oxynitrides and measurement conditions was demonstrated by evaluating previously reported chronoamperometries of oxynitride-based photoanodes.

Focusing on $LaTiO_2N$, a representative oxynitride, the degradation mechanism was investigated by systematically varying operational parameters, such as electrolyte composition, illumination or bias voltage and by conducting material characterization.

References:

[1] Schneidewind, J., Advanced Energy Materials, 2022. 12(18): p. 2200342.
[2] Vanka, S., et al.,. Frontiers in Energy Research, 2022. 10: p. 840140.
[3] Segev, G., et al., Journal of Physics D: Applied Physics, 2022. 55(32): p. 323003.
[4] Werner, V., et al., Progress in Solid State Chemistry, 2024. 73: p. 100442

Keywords: Photoelectrochemical water splitting, degradation, oxynitride

Optimizing fiber geometry in transparent fibrous conducting substrates for enhanced photoelectrochemical performance

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Abstract

Photon-driven electrochemical reactions typically involve photocatalysts deposited on top of planar conductive glass (SiO_2) substrates. Making the substrates fibrous can help improve the performance of the photoelectrochemical device since they increase the electrochemically active surface area and reduce the path length for charge carriers before they participate in redox reactions. However, the fibers also lead to optical losses due to scattering, reducing the transmittance of substrates and absorption of photons by the photocatalysts. In this study, a radiative transfer simulation model was developed to quantify the optical losses associated with fibrous substrates containing multi-layer coated fibers in order to optimize their design for reducing optical losses. The effect of fiber diameter, thickness of different layers, substrate porosity, and substrate thickness were investigated. It was found that minimizing optical loss required larger fibers and thin, highly porous substrates. The outputs from the simulation model can be incorporated into multi-physics models for the analysis of overall performance of photoelectrochemical cells containing porous fibrous photoelectrodes.

Keywords: ModVal2026, Photoelectrochemistry, Porous Media, Fibers, Optical Losses,

Predicting Operation and Degradation of Photoanodes

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Abstract

Stability issues hinder practical implementation of photoelectrochemical (PEC) devices for H_2 production [1]. Coupled physical modeling can elucidate photodegradation and aid the design of more stable devices but has only recently emerged [2]. Crucially, meaningful degradation modeling presupposes accurate reproduction of photoelectrode behavior across relevant operating conditions. Existing models, however, only focus on isolated aspects of the underlying physics, such as interfacial current-potential coupling [3], microkinetic charge-transfer modeling [4], or electrolyte mass transport [5].

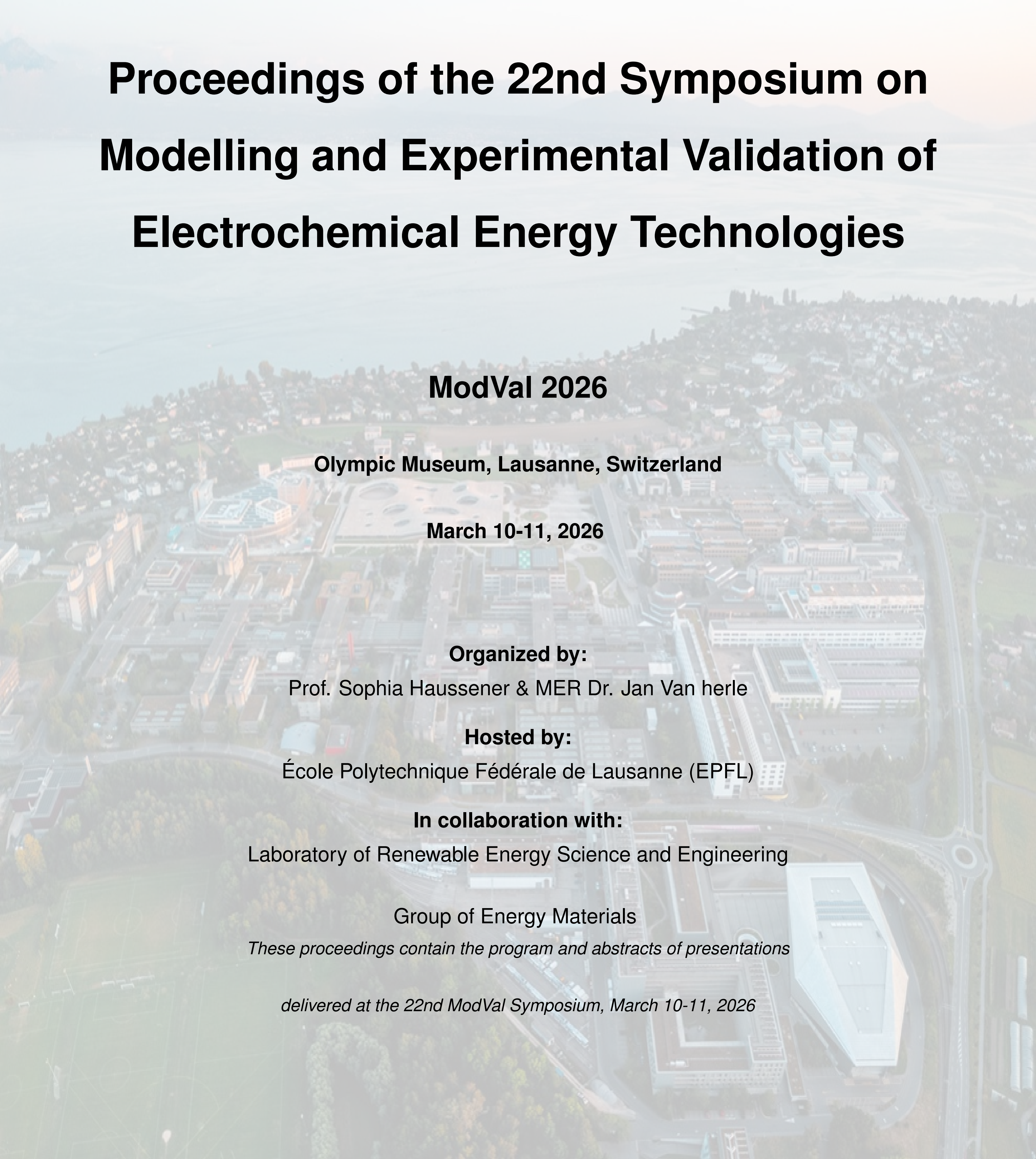
We present a one-dimensional photoanode-electrolyte model based on coupled charge-carrier dynamics that incorporates degradation phenomena. Charge transport in the photoanode and electrolyte is governed by drift–diffusion equations, with photogeneration and trap-assisted recombination in the photoanode and chemical equilibrium reactions in the electrolyte. Charge transfer across the PEI is mediated by surface states, incorporating band-edge shifts and a pH-dependent oxygen evolution reaction (OER) model. Distinct degradation mechanisms interfere differently with the OER, leading to transient changes in bulk and interfacial properties such as dissolution or surface passivation.

Applied to a naturally doped $BiVO_4$ photoanode in a phosphate-buffered electrolyte, the model accurately reproduces j–V curves across different operating conditions, including pH and solar concentration variations. Simulations varying absorber thickness and illumination direction reveal bulk transport limitations. Frequency-response and light-switching transients identify intrinsic material properties with distinct signatures, enabling robust parameter identification. Simulated Mott–Schottky analyses demonstrate limitations in extracting low dopant densities due to dominant carrier injection effects. Analysis of degradation fraction and current decay indicates that degradation pathways preceding the rate-determining OER step best reproduce experimental trends, suggesting surface transformation as a major contributor to $BiVO_4$ degradation besides dissolution.

The presented model simulates a broad range of experimentally accessible photoelectrode characteristics, including degradation-associated transient current decay. By linking device-level observables to underlying physical mechanisms, it enables mechanistic insight and provides guidance for PEC device optimization. The framework can be extended to multiple dimensions and complex photoelectrode structures, enabling analysis of heterogeneity and local operating-condition variations within PEC devices.

Keywords: PEC Water Splitting, Multiphysics Modeling, Degradation, $BiVO_4$

[1] J. Ager et al. (2015). *Energy Environ. Sci.*, 2015,8, 2811-2824
[2] F. Nandjou & S. Haussener (2022). *ACS Appl. Mater. Interfaces* 2022, 14,43095−43108.
[3] A. Iqbal & K. Bevan (2018). *J. Phys. Chem. C 2018*, 122, 30−43
[4] L.M. Peter (2025). *J Solid State Electrochem* 29, 2141–2155 (2025).
[5] F. Bedoya-Lora et al. (2017). *Journal of Materials Chemistry A*, 5(43):22683–22696, 2017.



Proceedings of the 22nd Symposium on Modelling and Experimental Validation of Electrochemical Energy Technologies

ModVal 2026

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March 10-11, 2026

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