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High-fidelity modeling of cell-level thermal runaway in lithium-ion batteries

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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
2026**

10-11 Mar, 2026
Lausanne, EPFL
Switzerland

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Program Overview

Tuesday March 10 th		
07:30	Registration opens at entrance of the museum	
08:45	Welcome, Room: <i>Auditorium</i>	
09:00	Plenary I, Room: <i>Auditorium</i>	
09:50	Short Break	
	Session A: <i>Energy Storage</i> Room: <i>Auditorium</i> (ground floor)	Session B: <i>Energy Conversion</i> Room: <i>Coubertin</i> (2 nd floor)
10:00	Session A1: <i>Next Generation</i>	Session B1: <i>High temperature electrolysis</i>
11:00	Coffee Break@Room Olympia, Poster@Room Olympia/Lausanne	
11:30	Session A2: <i>Thermal impact</i>	Session B2: <i>High temperature fuel cells</i>
12:30	Lunch Break@Room Olympia, Poster@Room Olympia/Lausanne	
13:40	Session A3: <i>Particle Cracking</i>	Session B3: <i>PEMFC I</i>
14:40	Coffee Break@Room Olympia, Poster@Room Olympia/Lausanne	
15:00	Poster Session 1@Room Olympia/Lausanne	
16:30	Session A4: <i>Diagnostics</i>	Session B4: <i>PEMFC II</i>
18:00	Poster Session@Room Olympia/Lausanne	
19:00	Conference Dinner at Olympic Museum	
Wednesday March 11 th		
08:30	Plenary II, Room: <i>Auditorium</i>	
09:20	Short Break	
	Session A: <i>Energy Storage</i> Room: <i>Auditorium</i> (ground floor)	Session B: <i>Energy Conversion</i> Room: <i>Coubertin</i> (2 nd floor)
9:30	Session A5: <i>Manufacturing</i>	Session B5: <i>PEMWE</i>
10:30	Coffee Break@Room Olympia, Poster@Room Olympia/Lausanne	
11:00	Session A6: <i>Modelling I</i>	Session B6: <i>AEMWE</i>
12:00	Lunch Break@Room Olympia, Poster@Room Olympia/Lausanne	
13:10	Session A7: <i>Modelling II</i>	Session B7: <i>Transport in electrodes and membranes</i>
14:30	Closing remarks and announcement of ModVal2027 at Room <i>Auditorium</i>	

Oral program

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

Tuesday March 10 th		
07:30	Registration opens at entrance of the museum	
08:45	Welcome, Room: <i>Auditorium</i> (ground floor) Chair: Sophia Haussener , Jan Van herle	
09:00	Plenary I, Chair: Sophia Haussener , Room <i>Auditorium</i> (ground floor) Curtis P. Berlinguette (University of British Columbia) <i>Reactive carbon capture</i>	
09:50	Short Break	
	Session A: Energy Storage Room: <i>Auditorium</i> (ground floor)	Session B: Energy Conversion Room: <i>Coubertin</i> (2 nd floor)
10:00	Session A1: <i>Next Generation</i> Chair: Jakub Wlodarczyk	Session B1: <i>High temperature electrolysis</i> Chair: André Weber
10:00	Siwar Ben Hadj Ali (Université de Picardie Jules Verne) An Experimentally-validated Modeling Workflow Coupling Electrochemistry and Solid Mechanics on Resolved Microstructures of ASSB Generated from Manufacturing	Andrey Koksharov (German Aerospace Center) Development of 3D Model for Proton Conducting Ceramic Electrolysis Cell
10:20	Nikolaos Papadopoulos (Porsche AG) Electrochemical Modeling of Silicon in Lithium-Ion Batteries Using a Multi-Species, Multi-Reaction Framework with Atomistic Insights	Meng Lin (Southern University of Science and Technology) Quantitative Analysis of Morphology and Performance of Electrode Microstructure in Solid Oxide Electrolysis Cells via Pore-scale Modeling
10:40	Elisa Buccafusco (Politecnico di Torino)	Yanyu Chen (Forschungszentrum Jülich GmbH)

	A Multiscale Numerical Investigation of LNMO/LFP Blended Cathodes	Multiphysics Simulation of Ni Agglomeration and Migration in Solid Oxide Cells under High-Steam Partial Pressure and Polarization Conditions
11:00	Coffee Break@Room Olympia, Poster@Room Olympia/Lausanne	
11:30	Session A2: <i>Thermal impact</i> Chair: Nicola Courtier	Session B2: <i>High temperature fuel cells</i> Chair: Meng Lin
11:30	Weihan Li (RWTH Aachen University) AI for Batteries: Modelling, Testing and Operation	Xinyu Guo (North China Electric Power University) Spatially-resolved local electrochemical performance of solid oxide electrolysis cell: the effects of steam supply and polarization
11:50	Mark Blyth (University of Bristol) Fitting Thermal Parameters from Electrical Data Gives Lumped Models of Heterogeneous Cells, by Predicting Their Effective Temperature	Felix Kullmann (Karlsruhe Institute of Technology) Design Guidelines for Ceria-based Fuel Electrodes: Connecting 3D Microstructure and Cell Performance
12:10	Sebastian Frentzen (Karlsruhe Institute of Technology) Degradation and Reformation of the Solid Electrolyte Interphase at the Onset of Thermal Runaway	Daniel Ewald (Institute for Applied Materials – Electrochemical Technologies) Impedance-based Performance Analysis and Modeling of Pressurized SOFCs for Aviation
12:30	Lunch Break@Room Olympia, Poster@Room Olympia/Lausanne	
13:40	Session A3: <i>Particle Cracking</i> Chair: Simon Daubner	Session B3: <i>PEMFC I</i> Chair: Fink Clemens
13:40	Maximilian Fath (Karlsruhe Institute of Technology) Quantifying the Impact of Secondary Particle Cracks on High-Nickel Insertion Batteries	Elisa Revello (Politecnico di Torino) Optimization of a hybrid battery-supported fuel cell propulsion architecture for a 4 MW regional aircraft
14:00	Philipp Benjamin Kuhn (Karlsruher Institute of Technology) Increased Effective Diffusion Coefficient of Secondary Particles Due to Beneficial Effects of Cracking	Fabian Klärchen (TU Braunschweig) Modeling of Liquid Water Transport in Fuel Cell Gas Channels Based on Contact Angles
14:20	Nikolai Erhardt (Karlsruher Institute of Technology) A Physics-Informed Model for Chemo-Mechanical Damage in Lithium-Ion Battery Particles	Maxence Desnoyers (Université de Picardie Jules Verne) Numerical Framework to Study Structural Wetting Properties of Proton Exchange Membrane Fuel Cell Catalyst Layers with Manufacturing Parameters

14:40	Coffee Break@Room Olympia, Poster@Room Olympia/Lausanne	
15:00	Poster Session@Room Olympia/Lausanne	
16:30	Session A4: <i>Diagnostics</i> Chair: Nikolaos Papadopoulos	Session B4: <i>PEMFC II</i> Chair: Jürgen Schumacher
16:30	Martino Fortunati (Politecnico di Milano) Machine Learning Model–Based Electrochemical Diagnostics for Comprehensive Lithium-Ion Battery Health Assessment	Yuze Hou (Fraunhofer Institute for Solar Energy Systems ISE) Pore-Scale Modeling of Through-Plane Reactive Transport in PEM Fuel Cell Electrodes with Optimized Mesoporous Carbon Supports
16:50	Quentin Moglia (Université Grenoble Alpes) Monitoring Heterogeneous Deformation in Lithium Batteries Using Strain Gauges and Digital Volume Correlation	Nikita Gusev (ETH Zürich) Lattice Boltzmann model for volume-averaged fluid dynamics in heterogeneous non-Darcian porous media
17:10	Priscilla Caliandro (Bern University of Applied Sciences) Battery Health Monitoring and Degradation Analysis for EV Fleets: A Data-Driven Pipeline Approach	Philipp Oppek (Karlsruhe Institute of Technology) Spatially Resolved Impedance Analysis and Modeling in PEMFCs
17:30	Noël Hallemans (University of Oxford) Multisine electrochemical impedance spectroscopy	Tancrede Oswald (Friedrich-Alexander Universität Erlangen-Nürnberg) Model-Based Reduction of the Required Validity Space of Electrochemical Models for Efficient Testing
18:00	Poster Session@Room Olympia/Lausanne	
19:00	Conference Dinner at Olympic Museum	

Wednesday March 11 th		
08:30	Plenary II, Chair: Jan Van herle , Room <i>Auditorium</i> (ground floor) Alejandro A. Franco (Unviersité de Picardie Jules Verne) <i>From Powder to Cell: Accelerating Battery Production with Multiscale Modeling, AI and XR</i>	
09:20	Short Break	
	Session A: Energy Storage Room: <i>Auditorium</i> (ground floor)	Session B: Energy Conversion Room: <i>Coubertin</i> (2 nd floor)
09:30	Session A5: <i>Manufacturing</i> Chair: Alejandro A. Franco	Session B5: <i>PEMWE</i> Chair: Roberto Valenza

09:30	Emmanuel Yerumoh (Université de Picardie Jules Verne) 3D Resolved Computational Modeling to Simulate the Electrolyte Wetting of a Lithium-Ion Battery Cell with 18650 Format	Lucas Anschütz (Leibniz University Hannover) Modelling Hydrogen Permeation during Run-in Phase of PEM Water Electrolysis
09:50	Caroline Willuhn (Technical University of Braunschweig) DEM-Based NCM622 Cathode Microstructures: Influence of Carbon-Binder-Domain Addition Method on Electrochemical Properties	Diamantis Almpantis (Lund University) Multiphysics and Data-Driven Modeling of AC-Coupled PV-PEM Systems with Experimental Validation
10:10	Simon Daubner (Imperial College London) Microstructure-aware DFN Models and the Tortuosity of Graded Electrodes	Felix Dittmar (Fraunhofer Institute for Chemical Technology) Development and Validation of a Layer-Unspecific Physical Model for Voltage Degradation and RUL Prediction in PEM Water Electrolyzers
10:30	Coffee Break@Room Olympia, Poster@Room Olympia/Lausanne	
11:00	Session A6: <i>Modelling I</i> Chair: Jakub Wlodarczyk	Session B6: <i>AEMWE</i> Chair: Matthieu Dessieux
11:00	Julian Ulrich (Karlsruhe Institute of Technology) Nonlinear Battery Model in Frequency-Domain and its Parameterization	Erwan Tardy (Université Grenoble Alpes) Modeling of Anion Exchange Membrane Electrolysis: Investigation of the Dual Ion-Transport Pathways
11:20	Max Okraschevski (German Aerospace Center) Towards a predictive scale-resolved 3D model of sulfurized polyacrylonitrile (SPAN) batteries for aviation	J.W. Haverkort (Delft University of Technology) Multiphase Flow Experiments and Modeling of Shunt Currents in Alkaline Water Electrolysers
11:40	Pierre Hugon (Université Grenoble Alpes) Quantification of Lithiation Heterogeneities in Graphite Electrode under Normal and Fast Charging Conditions Using Phase-field Modelling	Clemens Fink (AVL List GmbH) A Novel CFD Model for AEM Electrolyzers
12:00	Lunch Break@Room Olympia, Poster@Room Olympia/Lausanne	
13:10	Session A7: <i>Modelling II</i> Chair: Wolfgang Bessler	Session B7: <i>Transport in electrodes and membranes</i> Chair: Etienne Bountin
13:10	Patricia Ogochukwu Mmekwa (Offenburg University of Applied Sciences)	Christopher Arntsen (SINTEF Industry)

	Low-complexity Parameterization of a Degradation-sensitive Equivalent Circuit Model	Transport Properties of Ammonia-saturated Nafion Membranes
13:30	Mohammed Asheruddin Nazeeruddin (Imperial College London) Suppressing Phantom LAM/LLI in Voltage-Curve Degradation Mode Analysis via Ohmic IR Correction and Branch-Aware Hysteresis Handling	Tabea Schenuit (University of Stuttgart) Effective Reaction Rates of Oxygen Reduction Reaction in Gas Diffusion Electrodes by First Principles Microscale Modelling
13:50	Rabin Siva Dev (Mercedes-Benz AG) Modelling of OCV Hysteresis	Francesca Lorenzutti (École Polytechnique Fédérale de Lausanne) Pore-Scale Modeling of Electrochemical CO ₂ Reduction within the Catalyst Layer of a Gas Diffusion Electrode
14:30	Closing remarks and announcement of ModVal2027 at Room <i>Auditorium</i>	

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

Acknowledgments:

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References:

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3. Cellier, A., 2023. Simulation aux Grandes Echelles de Feux de Batteries Lithium-ion pour le Diagnostic de l'Emballage Thermique (Doctoral dissertation, Institut National Polytechnique de Toulouse-INPT).
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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*.