

# ModVal 2023

Symposium on Fuel Cell & Battery Modeling & Experimental Validation

21 - 23 March 2023 / Mercatorhalle - Duisburg, Germany

## PROGRAMME DAY 1

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### Sitetour (optional)

2:30 p.m.	Start at Mercatorhalle and transfer to ZBT by coach
3:00 p.m.	Presentation and tour of <b>ZBT - The Hydrogen and Fuel Cell Center</b>
4:30 p.m.	Transfer to Plug Power
5:00 p.m.	Presentation and tour of the European Headquarters of <b>Plug Power</b>
6:00 p.m.	Transfer to Mercatorhalle
6:30 p.m.	Drop-off at Mercatorhalle

### Welcome Dinner (optional)

7:00 p.m.	Dinner at Mercatorhalle
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Thank you,  
ModVal 2023  
Sponsors!



**MATH**  
2 MARKET

## PROGRAMME DAY 2

## PROGRAMME DAY 2

Room 4+5		Room 6	
8.00 a.m.		Registration	
9.00 a.m.	<b>Welcome</b> <b>Plenary Session I</b> Climate modelling: fundamentals, evaluation, and storyline simulations Helge Goessling	9.00 a.m.	
9.50 a.m.		Coffee break	
	<b>Battery degradation</b> Chair: Harry Hoster		<b>SOFC / SOEC / Methods</b> Chair: André Weber
10.20 a.m.	Modelling OER and HER in NiZn battery cells Britta Doppl	10.20 a.m.	Simulation of electrode diffusion models for solid oxide fuel cells Zhang Xiaoqiang
10.40 a.m.	Silicon-graphite composite electrodes: modelling state-of-charge and current distribution, and experimentally determining degradation rates Niall Kirkaldy	10.40 a.m.	Predicting the SOFC anode performance from microstructure using convolutional neural networks Pascal Plettenberg
11.00 a.m.	Simulation of Li plating in Si/Graphite composite electrodes Lioba Boveleth	11.00 a.m.	Multiscale and Multiphysics Modeling of an SOC Stack Zhang Shidong
11.20 a.m.	Monitoring battery degradation using acoustic signatures Elias Galiounas	11.20 a.m.	Modeling and simulation of an anion-exchange membrane electrolyzer using a unified open source platform for electrochemical systems Xavier Raynaud
11.40 a.m.	Health-aware battery fast charging optimisation Nicola E. Courtier	11.40 a.m.	Ontology-based graph data model for scalable data management in catalyst layer fabrication Max Dreger
12.00 p.m.		Lunch break	
	<b>Battery fabrication I</b> Chair: Ilona Glatt		<b>Redox flow batteries</b> Chair: Antoni Forner-Cuenca
1.10 p.m.	<b>KEYNOTE</b> 3D multiphysics model for large format lithium-ion cells and its application in an agile cell production André Weber	1.10 p.m.	<b>KEYNOTE</b> Advancing redox flow batteries through porous electrode and reactor engineering Antoni Forner-Cuenca
1.50 p.m.	A new approach for state of charge and state of health diagnosis of batteries using voltage-controlled models Wolfgang G. Bessler	1.50 p.m.	Starting from the bottom: Coupling a genetic algorithm and a pore network model for redox flow battery porous electrode optimization Maxime van der Heijden
2.10 p.m.	Pore-scale Modeling and Validation on the Calendaring of Lithium-Ion Battery Cathodes Xu Jie	2.10 p.m.	Optimizing electrode geometry for improved mass transfer in redox flow batteries: a CFD simulation and experimental study Michiel De Rop
2.30 p.m.	Modelling and experiments on porous electrodes with lithiated bin Tanmay Dev	2.30 p.m.	Combining electrochemical and imaging analyses to understand the effect of electrode microstructure and electrolyte properties on redox flow batteries Catalina A. Muñoz
2.50 p.m.	Electrode Structuring and its Effects on Battery Production and Performance Benjamin Kellers	2.50 p.m.	System-level performance modelling of regenerative fuel cells Ye Minnan
3.10 p.m.		Coffee break	
	<b>Data driven battery models</b> Chair: Nicola Courtier		<b>PEM-Systems / Degradation</b> Chair: Clemens Fink
3.50 p.m.	Battery Aging Identification Tool, a new Simcenter Amesim feature on electric storage library Rémy Mingant	3.50 p.m.	Modeling of Carbon Corrosion in PEM Fuel Cells applied to 3D Simulation Clemens Fink
4.10 p.m.	Machine learning for the classification of equivalent circuit models from solid-state electrochemical impedance spectra Joachim Schaeffer	4.10 p.m.	Simulating cathode catalyst morphology and degradation on porous carbon supports Anne-Christine Scherzer
4.30 p.m.	Operando EIS applied to commercial Li-ion batteries Noel Halleman	4.30 p.m.	Numerical modelling and simulation of metal interconnect oxidation of SOC stacks Yu Shangzhe
4.50 p.m.	Modelling Battery Behaviour with Physics informed neural Networks Josu Yeregui	4.50 p.m.	Investigation of scaled-down fuel cell system components by means of the IPEK X-in-the-loop approach Jan Haußmann
5.10 p.m.	Quantifying the impact of charge rate and number of cycles on particle cracking in Li-ion battery cathodes Orkun Furat	5.10 p.m.	Studies on Operational and Failure Dynamics of a Phase-Change Cooled Aviation PEM Fuel Cell System using Flownex® Gao Xin
5.30 p.m.		Poster session	
7.00 p.m.		Conference Dinner	

## PROGRAMME DAY 3

## PROGRAMME DAY 3

Room 4+5		Room 6	
All day		Poster exhibition	
9.00 a.m.	<b>Welcome</b> <b>Plenary Session II</b> Climate modelling: fundamentals, evaluation, and storyline simulations Gregory Offer		
9.50 a.m.		Coffee break	
	<b>Battery microstructure</b> Chair: Edwin Knobbe	<b>AEM, PEM and Alkaline Electrolysis</b> Chair: Moritz Pilaski	
10.20 a.m.	Li-ion battery in high C-rate conditions: improving the temperature prediction Volkan Kumtepe	10.20 a.m.	Multiphase zero-gap electrode simulations for alkaline water electrolysis Wouter Leen van der Does
10.40 a.m.	Microstructure-resolved simulation of three-dimensional electrodes for sodium iodine batteries Felix Gerbig	10.40 a.m.	CFD modeling of a PEM water electrolyzer: relationship between flow regime and performance Cheng Tianliang
11.00 a.m.	Understanding the Dynamics of Lithium-Ion Transport in Graphite-Silicon Composite Electrodes through Model Analysis Eduardo Jané	11.00 a.m.	Transient hydrogen crossover in dynamically operated PEM water electrolysis cells - a model-based analysis Tobias Franz
11.20 a.m.	Homogenized monolayers based 3D-model of a thermal event in a lithium-ion battery pouch cell Marcel Silas Tumelero	11.20 a.m.	Structure-performance relationship of IrO <sub>2</sub> nanoparticles during oxygen evolution: Investigation by dynamic microkinetic modeling Gözde Kardeş
11.40 a.m.	Multiphase-field modelling of layered-oxide compounds for intercalation batteries Simon Daubner	11.40 a.m.	Membrane electrode assembly simulation of anion exchange membrane water electrolyser Suhas Nuggehalli Sampathkumar
12.00 p.m.		Lunch break	
	<b>Battery fundamentals</b> Chair: Gregory Offer	<b>PEM / Microstructure I</b> Chair: Michael H. Eikerling	
1.00 p.m.	<b>KEYNOTE</b> Translating entropy measurements to next-generation battery materials Michael Mercer	1.00 p.m.	<b>KEYNOTE</b> Unraveling the role of ionomer and water in cathode catalyst layers of PEM fuel cells Michael H. Eikerling
1.40 p.m.	Electrode material design booster using a statistical digital twin Ilona Glatt	1.40 p.m.	Noninvasive local impedance determination in polymer electrolyte fuel cells stacks Jens Eller
2.00 p.m.	ENMR-derived Transference Numbers in Different Reference Frames Franziska Kilchert	2.00 p.m.	Experimental and modelling analysis of liquid water and current density distribution in a PEMFC stack Pierrick Balestriere
2.20 p.m.	Advances in LiS Model Validation and Prediction Michael Cornish	2.20 p.m.	Spatial Distribution of Loss Processes in PEMFC Philipp Oppek
2.40 p.m.	Why diffusion coefficients in active materials are not constants – On the importance of state-of-charge dependent input parameters in battery simulation Anja Bielefeld	2.40 p.m.	Electrochemical pressure impedance spectroscopy for PEM fuel cells: Model-based signal interpretation Lutz Schiffer
3.00 p.m.		Coffee break	
	<b>Battery fabrication II</b> Chair: Michael Mercer	<b>PEM / Microstructure II</b> Chair: Michael H. Eikerling	
3.30 p.m.	Cell design on target – maximum performance at optimal cost in minimal time Jan Richter	3.30 p.m.	Machine learning for the characterization of fibrous gas diffusion layers Dieter Froning
3.50 p.m.	Coupled EIS-FIB/SEM analysis of wet mixing effects on performance of Li-ion battery Saeed Abdolhosseini	3.50 p.m.	Multiscale simulation of nanostructured electrocatalytic systems by coupling neural network surrogates and continuum models Younes Hassani Abdollahi
4.10 p.m.	DEM-Simulation of Drying and Calendering of Lithium-Ion Battery Electrodes Carsten Schilde	4.10 p.m.	A coupled diffusion-mechanics model to investigate the interfacial mechanical damage at the microscale in block copolymer-based solid-state battery cathodes Soheil Bazazzadeh
4.30 p.m.	Identification of SEI growth models during Li-ion battery cell formation Felix Schomburg	4.30 p.m.	Advancement and validation of OpenFOAM PEMFC toolbox on automotive PEMFC design Sabina Schneider
4.50 p.m.		Closing	

Status: 21 March 2023