Lithium-Ion Batteries: Challenges and Opportunities

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Workshop Overview

Lithium-ion batteries permeate our lives. They are used in a wide range of products from portable electronic gadgets to electric vehicles and large container ships. These batteries are characterized by low costs, long life times, and high energy densities. With the increasing focus on shifting from fossil fuels to renewable energy sources, the demand for lithium-Ion batteries is expected to increase significantly in the next decade. Some projections estimate that the market for lithium-Ion batteries will increase from USD 41 billion in 2021 to USD 116 billion in 2030.

Despite their numerous advantages, there are several aspects of lithium-Ion batteries that are not fully understood. In particular, there is limited understanding of the internal electrochemistry, the aging process, and their ability to hold charge. Recent advances in battery design, modeling, and operations led to significant improvement in their safety and efficiency. In this workshop, we will introduce the attendees to battery design, modelling and estimation, and optimization of battery operation. The emphasis will be on using modern modeling/parameter estimation methods in conjunction with machine learning and optimization tools.

Learning outcomes:

By the end of this workshop, the attendees will:

1. Obtain an understanding of the internal processes and structure of lithium-ion batteries and its relationship with battery performance and state, such as state of charge and state of health
2. Know algorithms and software for building models, estimating parameters, and simulating battery charge/discharge cycles
3. Understand battery aging, and be able to estimate state of charge and state of health using state-of-the-art tools
4. Be able to optimize and control the operation of batteries
5. Obtain a good understanding of current challenges and opportunities in the battery industries

Expected Audience

Researchers, graduate students, and industrial practitioners interested in design and operation of lithium-ion batteries are the intended audience for this workshop.

List of Topics/Agenda

The following topics will be discussed in this workshop. Each topic will be accompanied by examples and case studies to highlight the practical relevance of the methods.

	Topic	**Speaker**	**Duration**
8:30 am –9:30 am	Model-Based Design and Analysis of Li-Ion Batteries From Cradle to Grave	Ulrike Krewer	60 min
9:30 am – 9:45 am	Discussion	All speakers	30 min
9:45 am – 10:00 am	Coffee Break		15 min
10:00 am – 11:00 am	Machine Learning-Based Model Identification an Prediction of Lithium-ion Batteries	Richard Braatz	60 min
11:00 am – 11:15 am	Discussion	All speakers	30 min
11:15 am – 12:15 am	Remaining Useful Life Prediction of Lithium-Ion Batteries: Applications to Electric Vehicles and Energy Management Systems	Jeesoon Choi	60 min
12:15 am – 12:30 am	Discussion		15 min
12:30 am – 1:00 pm	Lunch Break		30 min
1:00 pm – 2:00 pm	State of Charge and State of Health Estimation Method	Rolf Findeisen	60 min
2:00 pm – 2:15 pm	Discussion	All speakers	15 min
2:15 pm – 2:30 pm	Coffee Break		15 min
2:30 pm – 3:30 pm	Early Detection and Prediction of the Knee Point in Capacity Degradation of Li-ion Batteries Using Data-driven Methods	Jay H. Lee	60 min
3:30 pm – 3:45 pm	Discussion		15 min
3:45 pm – 4:45 pm	Model-Based Battery Management Systems: Optimal Charging Strategies	Davide Raimondo	60 min
4:45 pm – 5:00 pm	Discussion		15 min
5:00 pm – 5:30 pm	Panel Discussion – Challenges and Opportunities with Lithium-Ion Batteries	All speakers	30 min

Total time: 9 hr and 30 min including coffee breaks and lunch.

Speaker profiles:

Ulrike Krewer is Full Professor and Director of the Institute for Electrochemical Technologies at Karlsruhe Institute of Technology (KIT). Focus of her >20 years research is on model-based and dynamic analysis of electrochemical technologies from surface to cell level, with applications comprising various next-generation and established battery, fuel cell and electrolysis technologies. She received a Diploma in Process Engineering at the University of Erlangen-Nuremberg and a Ph.D. in Process and Systems Engineering at the University of Magdeburg. After applying her fuel cell knowledge in industry as Senior Researcher at the Energy Research Center of Samsung SDI, South Korea, she became Head of a research group on Portable Energy Systems at the Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, from 2008 to 2011, and Junior-Professor at the University of Magdeburg. She extended her research focus to Li-ion batteries in 2012 as Full Professor for Energy and Process Systems Engineering at Braunschweig University of Technology and board member of the Battery Labfactory Braunschweig and was a Visiting Scholar at the Massachusetts Institute of Technology before moving to KIT. She is Germany's regional representative of the International Society of Electrochemistry, member of the advisory board "Battery Research Germany", and chair of several international conferences and symposia on modeling of electrochemical systems.

Richard D. Braatz is the Edwin R. Gilliland Professor at the Massachusetts Institute of Technology (MIT) where he does research in applied mathematics and robust optimal control theory and its application to advanced manufacturing systems. He received an MS and a PhD from the California Institute of Technology and was a Professor at the University of Illinois at Urbana-Champaign and a Visiting Scholar at Harvard University before moving to MIT. His past professional service includes the Editor-in-Chief of IEEE Control Systems Magazine, the President of the American Automatic Control Council, General Chair of the IEEE Conference on Decision and Control and of the American Control Conference, and he is currently a Vice-Chair of the IFAC Conference Board. Honors include the AACC Donald P. Eckman Award, the Antonio Ruberti Young Researcher Prize, the IEEE Control Systems Society Transition to Practice Award, and best paper awards from IEEE- and IFAC-sponsored control journals. He is a Fellow of IEEE, IFAC, AIChE, and AAAS, and a member of the U.S. National Academy of Engineering.

Davide M. Raimondo received a Ph.D. in Electronics, Computer Science and Electrical Engineering from the University of Pavia, Italy, in 2009. From January 2009 to December 2010, he was a postdoctoral fellow in the Automatic Control Laboratory, ETH Zurich, Switzerland. From December 2010 to May 2015, he was assistant professor at University of Pavia. He has held visiting positions at the Massachusetts Institute of Technology, University of Seville, Vienna University of Technology, University of Konstanz. Prof. Raimondo is currently an associate professor and head of the educational Process Control Lab in the Department of Electrical, Computer and Biomedical Engineering at University of Pavia, Italy. He is the author or co-author of more than 100 papers published in refereed journals, edited books, and refereed conference proceedings. He serves as subject editor for the journals Automatica and IEEE Transactions on Control Systems Technology and served as CEB member of IEEE Control Systems Society. His current research interests include advanced battery management systems, set based estimation, fault diagnosis and fault-tolerant control, model predictive control and optimization. In 2017, Prof. Raimondo, with co-authors, received the 2014–2016 Automatica Paper Prize Award.

Rolf Findeisen received an M.S. from the University of Wisconsin–Madison, Madison, in 1997, and a Ph.D. from the University of Stuttgart, Stuttgart, Germany, in 2005. He was a Research Assistant with the Automatic Control Laboratory, ETH Zurich, Zurich, Switzerland, and a Researcher with the Institute for Systems Theory and Automatic Control, University of Stuttgart. He was a Full Chaired Professor and Head of the Systems Theory and Automatic Control Laboratory, Otto-von-Guericke University Magdeburg, Germany before moving to the Technical University of Darmstadt in 2021, where he heads the Control and Cyber-physical Systems Laboratory. He is the Chair of the IFAC Committee on Process Control and the IEEE Committee on Process Control and was the IPC Co-Chair of the 2020 IFAC World Congress.

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Jay H. Lee obtained a B.S. in Chemical Engineering from the University of Washington, Seattle, in 1986, and a Ph.D. in Chemical Engineering from California Institute of Technology, Pasadena, in 1991. Since, he is with the Chemical and Biomolecular Engineering Department at Korea Advanced Institute of Science and Technology (KAIST), where he was the department head from 2010 to 2015. He is currently KEPCO Chair Professor, and Director of the Saudi Aramco-KAIST CO_2 Management Center at KAIST. From 1991 to 2010, he held faculty appointments with Auburn, Purdue and then Georgia Tech. He was a recipient of the National Science Foundation's Young Investigator Award in 1993 and was elected as an IEEE Fellow and an IFAC (International Federation of Automatic Control) Fellow in 2011 and AIChE Fellow in 2013. He was also the recipient of the 2013 *Computing in Chemical Engineering* Award given by the AIChE's CAST Division and the 2016 Roger Sargent Lecturer at Imperial College, UK. He is currently an Editor of *Computers and Chemical Engineering* and also the chair of *IFAC Coordinating Committee on Process and Power Systems.* He published over 230 manuscripts in SCI journals with more than 18000 Google Scholar citations. His research interests are in the areas of system identification, state estimation, robust control, model predictive control, and reinforcement learning with applications to energy systems, bio-refinery, and CO_2 capture/conversion systems.

Jeesoon Choi currently serves as a Battery Modeling AI team leader in LG Energy Solution at the Battery Lab R&D Center. He obtained a B.S. in Mechanical Engineering from the Seoul National University (2010) and a Ph.D. in Mechanical Engineering from the California Institute of Technology (2016). He is a guest editorial board member of the IEEE Transactions on Transportation Electrification and he has been distinguished as a high-potential individual in LG Energy Solution. His research in data-driven battery modeling contributed to the emergence of a new business sector named the energy platform (e-Platform). Research interest includes data-driven battery modeling, reinforcement learning for longevity, optimal aging managements, quick charging and battery safety diagnostics.

Abstracts of Presentations:

Model-based design and analysis of Li-Ion Batteries – From Cradle to Grave
By Ulrike Krewer

Performance and durability of Li-ion batteries depend on confusingly many factors besides just selecting good materials. How do you structure and combine materials to get optimal battery designs? Then, once you operate a Li-ion battery, the cell is stressed in many ways, causing degradation, capacity and performance loss, and thus limited durability. But what is happening inside the battery during the cell's lifetime? How do materials change and what effect does this have? How can we diagnose its state? Finally, how can we be sure that it is still save to operate the battery, and what happens during a thermal runaway?

This talk shows how model-based analysis gets unprecedented insights into the underlying processes that cause the observed performance and degradation characteristics. The talk follows Li-ion batteries from cradle to grave. The first part elaborates on modeling methods and model-based insights of how to structure electrodes for high performance. The main part follows the Li-ion batteries from the first operation, during which a functional surface film in the nanometer range, the solid electrolyte interphase (SEI), is formed, via aging during operation to a final, spectacular death, i.e., the unwanted thermal runaway of Li-ion batteries.

The formation process of the SEI is analyzed using a coupled continuum-kinetic-Monte-Carlo model; it gives insight into the initial phase of film formation, where desorption of reactants hinders a rapid surface passivation, and the following phase where – depending on the applied current – different SEI compositions and structures are formed. It is further shown how during the lifetime of a battery, the degradation state including SEI thickness can be monitored by reproducing experimental impedance spectra with a continuum model. Further, nonlinear frequency response analysis is shown to be an essential additional diagnosis method to discriminate between aging types.

Eventually, an insight into the feared thermal runaway of batteries, i.e., the uncontrollable self-heating of batteries, is given with a physicochemical model and selected experiments. It reveals not only the crucial interaction of SEI decomposition, SEI formation reactions, and related phase changes, but it also highlights the notable impact of aging and impurities and allows to evaluate prevention strategies.

All in all, the model-based analysis not only gives a deeper, multiscale understanding of the processes in Li-ion batteries and the impact of design and operation on performance and degradation characteristics. It also opens the possibility for model-supported improvements of capacity, lifetime, and safety.

Machine Learning-based Model Identification and Prediction of Lithium-ion Batteries
By Richard D. Braatz

This presentation describes advances in machine learning-based techniques for addressing systems problems that arise for lithium-ion batteries. The specific systems problems include the prediction and classification of battery cycle lifetime (aka remaining useful life) and the identification of fundamental physicochemical expressions for electrochemical kinetics, thermodynamics, and mass transfer from real-time video imaging. The development of the techniques and their application are in collaboration with researchers at Stanford University, Toyota Research Institute, and MIT.

State of Charge and State of Health Estimation Methods
By Rolf Findeisen

Lithium-ion batteries are widely employed for energy storage in electrical vehicles, mobile devices such as smartphones, and house energy storage. They provide superior behaviors such as high energy density, long lifespan, and low self-discharge. Monitoring the state of charge and state of health subject to varying operational conditions, is however, essential for the operation of lithium-ion battery systems. Exact estimation and prediction of state of charge and state of health allows to optimally use – charge and discharge the battery - while avoiding degradation and possibly dangerous operational conditions. We provide a review of state of charge and state of health estimation methods, covering purely data driven, model based, and hybrid approaches. Focus is put towards online estimation methods, that allow an efficient operation in combination with cloud-based techniques.

Model-based Battery Management Systems: Optimal Charging Strategies
By Davide Raimondo

The battery management system (BMS) is a critical component of hybrid and electric vehicles. Its goal is to guarantee that the battery runs safely and reliably. One of the main tasks of the BMS is battery charging. Standard charging protocols, such as the Constant-Current-Constant-Voltage (CC-CV) and its variants, are usually based on excessively conservative constraints which reduce the probability of safety hazards at the expense of a longer charging time. Even so, constant voltage bounds, as in the CC-CV case, may not guarantee safety as the battery ages and its characteristics change. For these reasons, the research community has been interested in the development of BMSs which rely on mathematical models to increase the overall performance of the accumulators. This talk will focus on the key issues and challenges which arise when trying to design model-based battery management systems. In particular, we will focus on

1) Implementation of physics-based models for the simulation and control of single cells and battery packs: accuracy vs. complexity.
2) Parameter estimation of physics-based models: identifiability issues and uncertainty quantification.
3) Design of optimal aging-aware control charging strategies for lithium-ion cells and battery packs.

Early Detection and Prediction of the Knee Point in Capacity Degradation of Li-ion Batteries Using Data-driven Methods
By Jay H. Lee

Accurate monitoring of a lithium-ion battery degradation is important to take preemptive actions to minimize failures and plan battery replacement for optimal performance. Battery capacity fades with time due to repetitive charging and discharging until it reaches the onset of rapid degradation, which is called the 'knee point'. Batteries go through irreversible deterioration up to its end-of-life after the knee point, so it is crucial to forecast it for safety and economic benefits.

We discuss data-driven methods for online prediction of knee-point, ranging from a simple machine learning model based on manually extracted features to an application of convolutional neural networks (CNN) for automatic feature extraction. We evaluate several models and discuss the pros and cons of them. In addition, we present an analysis of the prediction results in relation to the underlying mechanism of battery degradation.

References

1. V. Laue et al., Joint Structural and Electrochemical Modeling: Impact of Porosity on Lithium-ion Battery Performance, Electrochimica Acta 314, 20-31, 2019

2. D. Witt et al., Myth and Reality of a Universal Lithium-Ion Battery Electrode Design Optimum: A Perspective and Case Study, Energy Technology, 2000989, 2021

3. F. Röder et al., Model Based Multiscale Analysis of Film Formation in Lithium-Ion Batteries, Batteries & Supercaps 2 (3), 248-265, 2019

4. F. Röder et al., Multi-Scale Simulation of Heterogeneous Surface Film Growth Mechanisms in Lithium-Ion Batteries, Journal of The Electrochemical Society 164 (11), E3335-E3344, 2017

5. M. Heinrich et al., Physico-Chemical Modeling of a Lithium-Ion Battery: An Ageing Study with Electrochemical Impedance Spectroscopy, Batteries & Supercaps 2 (6), 530-540, 2019

6. K. A Severson, et al. Data-driven prediction of battery cycle life before capacity degradation. Nature Energy, 4:383-391, 2019.

7. M. D. Berliner et al. Methods-PETLION: Open-source software for millisecond-scale porous electrode theory-based lithium-ion battery simulations. Journal of The Electrochemical Society, 168(9):090504, 2021.
8. M. Aykol et al. Perspective—Combining physics and machine learning to predict battery lifetime, 168(3):030525, 2021.
9. Pozzi, A. and Raimondo, D.M. Optimal Control and Reinforcement-Learning Strategies for Advanced Management of Lithium-Ion Battery Packs, 2021.
10. Campbell, I.D et al. Optimising lithium-ion cell design for plug-in hybrid and battery electric vehicles. *Journal of Energy Storage*, *22*, pp.228-238.