Welcome to Oxford!

You are warmly welcomed to the inaugural Oxford Battery Modelling Symposium. Enthusiasm for the topic of battery energy storage continues to grow at an ever-increasing pace. Indeed, it was recently estimated that car companies are planning to spend the eye-watering amount of $300 billion on electric vehicle technology over the next 5-10 years\(^1\). Here in the UK, the government has recently committed £246 million to battery research, including the establishment of the Faraday Institution, a new independent organisation for electrochemical energy storage science and technology.

There are many excellent battery conferences around the world, but we decided to organise this event specifically to bring together the modelling community, which is a relatively smaller subset of the wider battery research community. We have been overwhelmed by the response, and are delighted that 170 participants are attending, from a wide range of universities, companies, and research organisations internationally. The program includes 13 oral presentations from world-renowned experts, as well as a poster session with 25 posters. Abstracts for all speakers (pp. 3-15) and posters (pp. 16-38) may be found in this booklet. Over the two days, we begin at the atomistic length scale and then travel up to continuum models and finally to control-oriented approaches.

Oxford University is the oldest university in the English-speaking world, founded in the 12\(^{th}\) century. The University has a federal structure comprising 38 self-governing colleges in addition to various centralised departments and institutes. Pembroke College, the location of this symposium, was founded in 1624. Oxford has a long association with battery research; in fact it was here in 1980 at the Inorganic Chemistry Laboratory on Parks Road that John Goodenough and colleagues identified the cathode material that subsequently enabled the development of lithium-ion batteries.

We would like to express our appreciation to the events team at the Department of Engineering Science who have worked hard to make this event happen, particularly Clem Hadfield. We are also grateful to Comsol Ltd. and to the UK’s EPSRC-supported Materials Research Hub for Energy Conversion, Capture, and Storage (M-RHEX) for sponsorship of the poster session. COMSOL is a global provider of multiphysics simulation software for product design and research; please visit their display table at the symposium. M-RHEX brings together a team of internationally-leading researchers from a range of disciplines for a research programme aimed at advancing the fundamental science of charge mobility.

We hope that you enjoy your time here and find the symposium inspiring and useful.

Organising committee of the Oxford Battery Modelling Symposium:

David Howey (Department of Engineering Science)
Charles Monroe (Department of Engineering Science)
Jon Chapman (Mathematical Institute)
Colin Please (Mathematical Institute)

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\(^{1}\) https://uk.reuters.com/article/uk-autoshow-detroit-electric-exclusive/exclusive-vw-china-spearhead-300-billion-global-drive-to-electrify-cars-idUKKCN1P40GI
**PROGRAM**

(Abstracts are available on pages 3-15 in order of presentation)

**Day 1 – Monday 18th March 2019**

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<td><strong>Session 1: Atomistic to continuum modelling (chair Jon Chapman)</strong></td>
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<td><strong>Anton Van der Ven</strong> – “Connecting electronic structure to phenomenological continuum models of electrochemical processes”</td>
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<td>11:00</td>
<td><strong>Denis Kramer</strong> – “Mind the Gap – Towards an atomistic understanding of battery materials interfaces”</td>
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**Day 2 – Tuesday 19th March 2019**

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<td><strong>Martin Bazant</strong> – “Control of battery phase transformations by electro-autocatalysis”</td>
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<td><strong>Göran Lindbergh</strong> – “An extended porous electrode model for NMC111 in lithium-ion batteries”</td>
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Connecting electronic structure to phenomenological continuum models of electrochemical processes

Anton Van der Ven
University of California Santa Barbara

Abstract: Most electrochemical processes can be modeled with powerful phenomenological theories that describe ion transport, interface reactions and mechanical responses. Phenomenological descriptions, however, rely on materials specific coefficients and potentials, some of which may be difficult to measure in isolation. An alternative to an experimental approach is to predict these quantities from first principles. Since electrochemical processes are thermally activated, temperature and entropy play an important role. The prediction of materials properties, therefore, requires a statistical mechanics approach. In this talk I will describe a generalized framework with which to connect the electronic structure of crystalline solids to their equilibrium and kinetic properties at the macroscopic scale. I will illustrate how the application of first-principles statistical mechanics can generate crucial ingredients for phenomenological models of electrochemical processes, including composition dependent free energies and open circuit voltage profiles, ionic transport coefficients and chemo-mechanical response functions. The capability to predict thermodynamic and kinetic properties of electrode materials is allowing us to explore and design new battery chemistries and concepts. Electrode materials for Li, Na and Mg ion batteries undergo a series of phase transformations as a result of large changes in concentration during each charge and discharge cycle. While the mechanisms of these phase transformations remain poorly characterized they can to an extent be understood with first-principles approaches.

Biography: Anton Van der Ven is Professor of Materials at the University of California Santa Barbara. His research seeks to unravel the links between the electronic structure of solids and their macroscopic properties using first-principles statistical mechanics. He studies a wide variety of materials classes for electrochemical energy storage and high temperature aerospace applications. He has spent almost two decades investigating the unique electronic, thermodynamic and kinetic properties of transition metal oxides and sulfides used as electrodes in Li-ion batteries. His group develops statistical mechanics methods and accompanying software tools to predict the properties of complex crystals from first principles. Van der Ven studied metallurgy at the Katholieke Universiteit Leuven, Belgium, and obtained a PhD in Materials Science at the Massachusetts Institute of Technology.
Mind the gap – towards an atomistic understanding of battery materials interfaces

Denis Kramer

University of Southampton

Abstract: How can one rigorously capture the real behaviour of battery materials and interfaces in models and theories? Whilst we have astonishingly accurate atomistic models to describe materials and well developed sets of idealised continuum theories, we generally lack rigorous ways to connect the two and construct non-ideal continuum descriptions from first principles. Physically rigorous models, however, are essential to describe real battery characteristics with confidence and predictive power. Merely describing the experimentally observed behaviour is generally insufficient to drive design and optimisation. Truly powerful battery models predict beyond the experimentally readily accessible: they allow the exploration of extreme or out-right dangerous operating conditions, the evolution of properties over the full service life including end-of-life, the exploration of novel combinations of chemistries, manufacturing routes and engineering designs. I will start out reviewing successful (and failed) contributions of First Principles theory to electrochemical technologies establishing the utility and predictive power available at the atomistic length-scale, followed by outlining strategies to rigorously construct continuums theories from atomistic descriptions and present selected case studies.

Biography: Denis Kramer is Associate Professor within the Faculty of Engineering and Physical Sciences at the University of Southampton. He graduated with a Dipl.-Ing. (FH) from the University of Applied Sciences Zwickau (Germany) in 2002; was awarded a PhD in Mechanical Engineering (summa cum laude) from the Technical University in Freiberg (Germany) in 2007 for his work on "Mass transport aspects of Polymer Electrolyte Fuel Cells under Two-Phase Flow Conditions" carried out at the Electrochemistry Laboratory of the Paul Scherrer Institut (Switzerland). Being awarded a Fellowship of the German Academic Exchange Service, he spent two years at the Massachusetts Institute of Technology (USA) studying Li-ion batteries based on Density-Functional-Theory with Gerbrand Ceder. He relocated to the UK in 2009 working with Anthony Kucernak at Imperial College London. He joined the University of Southampton in 2011. His research interests focus on electrochemical energy conversion technologies such as fuel cells and batteries. He mainly works at the interface between theory and experiment, combining state-of-the-art computational materials design (based on DFT) with advanced electrochemical characterisation and synthesis techniques to discover technology-enabling materials for these devices. His current interests include the electrochemistry of oxide surfaces, the thermodynamics of nanoscale systems, phase stability of multi-component systems in aqueous environments, and fundamental aspects of electro-kinetic processes. He is Co-Director of the EPSRC CDT in Next-Generation Computational Modelling, received the "Christian Friedrich Schönbein" Contribution to Science Medal in 2005, and a RAEng/Leverhulme Trust Senior Research Fellowship in 2016. He published 35+ papers that attracted more than 2300 citations so far.
Modeling porous intercalation electrodes with continuum thermodynamics and multi-scale asymptotics

Manuel Landstorfer

Weierstrass Institute for Applied Analysis and Stochastics

Abstract: This talk will give an overview of the modelling procedure of porous intercalation electrodes on the basis of non-equilibrium thermodynamics and multi-scale asymptotics. Within a porous battery electrode, at least three scales arise: the macroscopic porous media scale, the micro-structure scale, and the double layer scale. Each of these scales fundamentally contributes to the overall performance of a battery cell, and several strategies exists to overcome the scales in a mathematical model [1-4]. I will sketch the modelling of the double layer scale with non-equilibrium thermodynamics [5] and the upscaling to the electrode particle scale with matched asymptotic expansions [6]. Some thermodynamic aspects are discussed [7], as well as material models for the intercalation phase, before we proceed to the next scale. Homogenization techniques are employed to deduce the transport equations for the porous media scale as well as the geometric cell problem for the micro-structure [8-9]. The later allows to determine porosity, tortuosity and interfacial area based on real micro-structure models [10]. For various material models of the intercalation phase we discuss some aspects of the open circuit potential on the porous media scale [10]. Numerical simulations show the validity of the overall approach, and potential extensions regarding ageing effects are finally discussed.

References

Biography: Manuel Landstorfer received his Ph.D. in Mathematics from Ulm University (Prof. S. Funken, Prof. T. Jacob) in 2013. Since then he is research associate at the Weierstrass Institute for Applied Analysis and Stochastics (WIAS) in Berlin. His research focuses on modelling electrochemical systems with continuum non-equilibrium thermodynamics. Together with W. Dreyer and C. Guhlke he studied extensively electrochemical interfaces, especially the double layer and electro-capillary effects in the last years. A very important aspect of his work is model validation. More recently he focuses on homogenization techniques for porous electrochemical cells. Applications in this topic range from fundamental electrochemistry to batteries and electrolysers, and quite recently he became head of a joint BMBF-project dealing with ageing effects in lithium ion batteries.
Electrochemical energy storage

John Newman

University of California Berkeley

Abstract: Storing renewable energy at a competitive cost makes that energy dispatchable and comparable to fossil fuels. Achieving low cost electrochemical energy storage is one of the most difficult technical and manufacturing challenges of our time. Batteries exist to store energy and deliver it at high power and energy. Mathematical models based on physical laws can be used to design batteries for specific applications. Such models can predict and optimize performance and elucidate failure mechanisms and other limitations such as safety, life, and cost. Because batteries are expensive and cannot always meet performance requirements, there is always a search for better materials for electrodes, separators, and electrolytes. Results from mathematical modeling of battery systems are discussed in the context mentioned above.

Biography: John Newman is a retired Professor of Chemical Engineering at the University of California, Berkeley, and Faculty Senior Scientist at Lawrence Berkeley National Laboratory. He has been a Principal Investigator at LBNL with the DOE Batteries for Advanced Transportation Technologies Program. He is the author or co-author of more than 400 technical publications, numerous plenary and invited lectures, and the book Electrochemical Systems. Prof. Newman has received many awards, was an Onsager Professor at the Norwegian University of Science and Technology in Trondheim in 2002; and was elected to the National Academy of Engineering in 1999.

Professor Newman’s research focuses on the analysis and design of electrochemical systems, with special emphasis on batteries and fuel cells. In more recent years he has shown an interest in renewable energy and in turbulence.

Additional details about Professor Newman and his research group can be found at http://www.cchem.berkeley.edu/jsngrp/
Modeling of high-energy-density graphite electrodes

Charles Delacourt

CNRS Researcher, Laboratoire de Réactivité et de Chimie des Solides, UMR 7314, Université de Picardie Jules Verne, 33 Rue Saint Leu, 80039 Amiens cedex, France

Abstract: The Li-ion battery is the energy-storage technology that is used in the majority of today’s electric vehicles (EVs). This is thanks to its high energy density along with long lifetime, compared with other battery technologies. Still, EV market penetration is made difficult both by the limited battery performance, which limits vehicle mileage, and by the battery performance decay over time, which limits vehicle service life. Physics-based modeling is quite powerful in order to understand performance limitations of an actual battery under specified usage. It is also possible to predict the occurrence of degradation phenomena, such as Li plating during charge. This type of modeling is well-suited to aid in cell design, by readily answering a number of “what-if” questions aiming at finding an optimum for performance (energy/power) while preventing side effects from happening.

In this presentation, we will concentrate on a modeling-based study of a set of industry-grade graphite electrodes with different designs, ranging from ca. 25 to 120 µm in terms of thickness and ca. 12 to 45% in terms of porosity. Specific model experiments and data analysis were developed for measuring input parameters such as electrode tortuosity [1], and particle-related parameters such as Li insertion rate constant and solid Li diffusion coefficient [2]. Once all input parameters were determined, electrode performance was simulated for the full set of electrodes and was shown to agree with corresponding experimental measurements without any parameter adjustment [3]. This calibrated model was subsequently used for predicting Li plating conditions for the full set of electrodes.

References

Biography: Charles has been a CNRS researcher at Laboratoire de Réactivité et Chimie des Solides (France) since 2007. He completed his PhD in materials chemistry at Université de Picardie Jules Verne (Amiens, France), in 2005. He was then a Postdoctoral fellow for two years in Prof. John Newman’s group at University of California, Berkeley. Charles has authored nearly 56 peer-reviewed papers and 3 patents, and got awarded several distinctions, among which the "Carl Wagner Medal of Excellence in Electrochemical Engineering of the European Federation of Chemical Engineering" (2011) and the "Oronzio and Niccolò De Nora Foundation Prize of ISE on Applied Electrochemistry" (2009). Current effort is the development of physics-based mathematical models for studying lithium-ion batteries, with a focus on electrolyte transport properties and battery degradation. His research is in close collaboration with French automotive industry.
Redox kinetics, interface roughening and solid electrolyte cracking in solid state lithium-ion batteries

Robert McMeeking

University of California Santa Barbara

Abstract: A model is developed for the redox kinetics at an interface between a single ion conducting solid electrolyte and a lithium metal anode with inclusion of the effect of the mechanical stress across the interface, thereby extending the Butler-Volmer equation. This formulation is then used to assess the morphological stability of sinusoidal roughness on the surface of the lithium metal electrode when it is being plated from the single ion conducting solid electrolyte, to which it is bonded. It is assumed that the lithium responds elastically and does not yield plastically. It is found that long wavelength roughness exceeding a critical value will always grow in amplitude. The critical value of the wavelength is proportional to the elastic shear modulus of the electrolyte, and inversely proportional to the current density in and the resistivity of the solid electrolyte. Therefore, any wavelength of roughness can be induced to increase in amplitude if the current density is high enough. The extended Butler-Volmer equation is also used to assess cracking of the solid electrolyte caused by insertion of lithium into a pre-existing flaw. It is found that lithium insertion from the solid electrolyte into the pre-existing flaw causes the lithium to yield plastically, and that pressure in the lithium in the crack builds up very rapidly. This pressure can cause the crack to propagate, thereby inducing dendrite growth that can short circuit the cell. This will occur unless the pressure in the lithium in the crack blocks the redox reaction that is inserting the lithium into it. This possibility is investigated by use of the extended Butler-Volmer equation. In addition, the question of whether the lithium can extrude from the crack into the lithium electrode is investigated. It is found that it is likely that the lithium is contained within the crack, thereby enabling it to propagate the dendrite-flaw.

Biography: Robert McMeeking earned a BSc in Mechanical Engineering with First Class Honours at the University of Glasgow, Scotland in 1972. He completed his Ph.D. in solid mechanics at Brown University in 1976 and then was Acting Assistant Professor at Stanford University for 2 years. Thereafter he joined the faculty of the Theoretical and Applied Mechanics Department in the University of Illinois at Urbana-Champaign. He moved to UCSB in 1985 as Professor of Materials and of Mechanical Engineering, and was Chair of the Department of Mechanical Engineering 1992-1995 and again during 1999-2003. McMeeking is currently Tony Evans Distinguished Professor of Structural Materials and Distinguished Professor of Mechanical Engineering at UCSB. He is also Sixth Century Professor of Engineering Materials at the University of Aberdeen in Scotland and Leibniz Professor at the Leibniz Institute for New Materials in Saarbrücken, Germany. He has published approximately 300 papers on a variety of subjects in the mechanics of materials area. McMeeking was Editor-in-Chief of the Journal of Applied Mechanics from 2002 to 2012, and is currently Secretary of the Congress Committee of the International Union of Theoretical and Applied Mechanics and President of the International Congress on Fracture. He is a member of the U.S. National Academy of Engineering, Fellow of the American Society of Mechanical Engineers, Fellow of the U.K. Royal Academy of Engineering and Fellow of the Royal Society of Edinburgh. He held a Humboldt Award for Senior Scientists in 2006, again in 2013, and received a Humboldt Alumni Award in 2018. He was given the Brown Engineering Alumni Medal in 2007, the 2014 William Prager Medal of the Society of Engineering Science, and the 2014 Timoshenko Medal of the American Society of Mechanical Engineers. In 2018 McMeeking was awarded the honorary degree of Doctor of Engineering by the University of Glasgow.
Control of battery phase transformations by electro-autocatalysis

Martin Bazant

Massachusetts Institute of Technology

Abstract: The rapid, stable cycling of rechargeable batteries requires well-controlled phase transformations of the redox active materials in each electrode, between the charged and discharged states. In Li-ion batteries, common intercalation materials, such as graphite and iron phosphate, undergo phase separation (into Li-rich and Li-poor phases), which limits the power density and causes degradation, and unusual high-rate “phases” have also been reported in solid-solution NCM layered oxides. A general stability theory will be presented for single particles [1] and populations in porous electrode [2,3], based on electrochemical non-equilibrium thermodynamics [4], which accurately predicts the driven phase behavior revealed by x-ray imaging [5,6]. Interfacial stability is strongly influenced by the asymmetric dependence of the exchange current on concentration (“electro-autocatalysis”).

References

Biography: Martin Z. Bazant is the E. G. Roos (1944) Professor of Chemical Engineering and Mathematics and Executive Officer of the Department of Chemical Engineering at the Massachusetts Institute of Technology. After a PhD in Physics at Harvard (1997), he joined the MIT faculty in Mathematics (1998) and then in Chemical Engineering (2008). His research focuses on electrokinetics, electrochemical systems, and applied mathematics. He is a Fellow of the American Physical Society, the International Society of Electrochemistry and the Royal Society of Chemistry. His awards include the 2015 Kuznetsov Prize in Theoretical Electrochemistry (ISE) and 2018 Andreas Acrivos Award for Professional Progress in Chemical Engineering (AIChE). He also serves as the Chief Scientific Advisor for Saint Gobain Ceramics and Plastics, North America.
An extended porous electrode model for NMC111 in lithium-ion batteries

Professor Göran Lindbergh

KTH Royal Institute of Technology

Abstract: The objective is to show how an extended physics-based porous electrode model accounting for particle surface stress can be used to describe the electrode kinetic performance of NMC111 in lithium-ion batteries. The electrodes are experimentally investigated using galvanostatic intermittent titration technique (GITT). Due to the unsuccessful description of the electrochemical behaviour by the standard models, an extended pseudo-two-dimensional (P2D) model is developed to extract transport, kinetic, thermodynamic and stress properties. A stress proportionality factor is derived that depends on the build-up of lithium concentration gradients in the particles, and that can explain the slow relaxation phenomena seen during GITT pulses. Four physical parameters are optimized from the model fitting and their dependency on the electrode potential and temperature is studied. Two regions of different behaviours can be identified: less particle surface stress and better diffusion at potentials up to ~3.8 V, and high surface stress and slow solid-phase diffusion from ~3.8 to 4.1 V.

Biography: Göran Lindbergh has both an MSc (1985) and PhD (1991) in Chemical Engineering from KTH Royal Institute of Technology, Stockholm, Sweden. He is Professor in Electrochemical Process and System Engineering at KTH since 2003, and was heading the Department of Chemical Engineering between 2005 and 2017. He is also a member of The Royal Swedish Academy of Engineering Sciences (IVA) and coordinating the energy storage activities in the Swedish Electromobility Centre. He has more than 190 published journal papers. He is leading the Applied Electrochemistry group at the Department of Chemical Engineering working with electrochemical power sources and electrolytic processes within the field of electrochemical engineering. A common theme in the on-going research projects is the mathematical modelling and electrochemical characterization of batteries and fuel cells.
Physically-informed models for improved cell design and operation of lithium-sulphur cells

Dr Monica Marinescu
Imperial College London

Abstract: In order to create better performing battery systems, one can improve the cell chemistry, but also all the engineering that links component materials behaviour to the device and battery pack performance. Certain types of battery models can be used as powerful tools in detecting the mechanisms that limit operation. This information, in turn, can be used to create superior battery cells, battery packs and battery management systems. Relatively simple physics-derived models can be created from the description of only those mechanisms that are potentially dominating a battery’s performance. I will show how such models have delivered essential knowledge for commercially-sized lithium-sulphur batteries, such as identifying the probable main causes of discharge rate limits [1], charge rate limits [2], and decoupling their memory effect from irreversible degradation [3]. Early modelling work applying the same philosophy to Li-ion batteries will also be presented, that highlights the importance of minimising temperature gradients across parallel layers in a cell, and identifies the bottlenecks in the thermal paths inside a cell [4].

References

Biography: Dr Monica Marinescu received her PhD in Physical Chemistry from Imperial College London in 2012. Since then, she has been working on continuum and reduced order models of lithium-ion batteries, lithium-sulphur batteries, supercapacitors, and Li-ion capacitors. Her research focuses on determining the physical and chemical mechanisms that limit the performance of energy storage devices in real applications, and developing the models that can help design better cells and help use those cells to their fullest potential. She is particularly interested on how knowledge of the load cycle can inform cell design and control.
A Padé approximant model of lithium ion batteries

Professor Troy Farrell
Queensland University of Technology

Abstract: We present a reduced order model for a lithium ion battery in which Padé approximants are used to simplify complicated transcendental transfer functions associated with the linearized, pseudo 2-dimensional (P2D) electrochemical model of the battery. The resulting transfer functions take the form of simple rational polynomial functions, which can be used to compute any variable at any location within a one-dimensional representation of the battery domain. Corrections for nonlinear behaviour are also incorporated into the reduced model. The results from our reduced model are shown to compare favourably to those from the full (nonlinear) P2D model and the computational time required to produce these results is significantly reduced. We also consider an application of the Padé approximant model to large format, cylindrical lithium ion batteries in which thermal and degradation effects are coupled to the model.

Biography: Troy Farrell received his PhD in applied mathematics from Queensland University of Technology (QUT) in 1999 and is currently a Professor in Applied and Computational Mathematics there. His research interests are in industrial applications including batteries and electrochemical devices. He has worked with several battery and battery materials manufacturers to develop multiscale, multiphysics, simulation models for primary and secondary battery chemistries. In recent times he has become interested in battery storage systems for grid-scale, renewable energy generation. This work centres on the development of accurate and computationally efficient, physics-based, reduced order models for use in battery management systems.
Physics-based reduced-order models of lithium-ion cells for battery management systems

Gregory Plett
University of Colorado, Colorado Springs

Abstract: Battery-management systems are required to compute continuous estimates of state-of-charge, state-of-health, available energy, and available power. Traditional methods to accomplish these objectives rely on empirical equivalent-circuit models of battery cells. These models can enable sufficient accuracy for many of these tasks, especially for new lithium-ion cells, but they cannot predict the internal electrochemical state of the battery cell. Knowledge of this internal state is needed to compute a direct trade-off of life versus performance, since the rate of aging depends directly on the internal electrochemical state and not on cell terminal voltage (which is what is presently assumed). Physics-based models are able to provide good predictions of the internal electrochemical state, but standard models are too complex to run on a battery-management system. Methods are needed to reduce the computational requirement of these physics-based models while retaining their prediction accuracy. This talk will review the standard physics-based model, show how the model can be converted to a reduced-order equivalent using standard linear-algebra and signal-processing methods and show results comparing predictions made by the full-order physics-based model to those made by the reduced-order models.

Biography: Professor Plett received his Ph.D. in Electrical Engineering from Stanford University in 1998. Since then, he has been on the faculty of the Department of Electrical and Computer Engineering at the University of Colorado, Colorado Springs. His research focuses on control-systems theory as applied to the management of high-capacity battery systems, such as found in hybrid and electric vehicles. Current research efforts include: physics-based reduced-order modeling of ideal lithium-ion dynamics; system identification of physics-based model parameters using only current-voltage input-output data; physics-based reduced-order modeling of degradation mechanisms in electrochemical cells; estimation of cell internal state and degradation state; state-of-charge, state-of-health and state-of-life estimation; power and energy prediction; and battery pack fast charging.
Decoding the electrode swelling for advanced battery diagnostics

Anna Stefanopoulou
University of Michigan

Abstract: The battery management system (BMS) relies on accurate prediction of complex electrochemical, thermal and mechanical phenomena. This raises the question of model and parameter accuracy. Moreover, if the cells are aging, which parameters should we adapt after leveraging limited sensor information from the measured terminal voltage and sparse surface temperatures? With such a frugal sensor set, are there driving or charging patterns that improve the parameterization confidence levels? To this end, observations of the cell swelling during charging will be used for higher confidence and even for estimating the Loss of Active Material (LAM) and Loss of Lithium Inventory (LLI) in the anode, which is useful for avoiding Li-plating during fast charge. We will conclude by highlighting the fundamental advantages of mechanical measurements in estimating the onset of thermal runaway due to an internal short circuit.

Biography: Prof. Anna Stefanopoulou is the William Clay Ford Professor and the Director of the Energy Institute at the University of Michigan. She was an assistant professor at the University of California, Santa Barbara and a technical specialist at Ford Motor Company. She is an ASME (08), an IEEE (09) and a SAE (18) fellow, an elected member of the Executive Committee of the ASME Dynamics Systems and Control Division and the Board of Governors of the IEEE Control Systems Society. She has received multiple awards and two involving battery state estimation using mechanical (swelling) behavior.
Model predictive control using physics-based models for advanced battery management

Scott Trimboli
University of Colorado, Colorado Springs

Abstract: Physics-based models (PBM) of lithium-ion batteries can describe internal cell behavior with surprising accuracy. Recent advances in subspace-based model-order reduction enable these often highly complex, nonlinear electrochemical models to be rendered into forms no more demanding than familiar equivalent circuit models, and therefore make them candidates for embedded battery management schemes. Model predictive control (MPC) has recently emerged as an effective real-time control strategy that employs a ‘look-ahead’ approach to foresee dynamic behaviors before they happen. This approach – when coupled with an ability to enforce hard constraints on internal electrochemical variables that are precursors to degradation or unsafe operation – makes MPC particularly appealing for advanced battery management, where safety, lifetime and improved performance are key. This presentation will introduce the basics of MPC and illustrate the potential improvements in battery management that may be achieved by combining reduced-order PBM’s of lithium-ion cells with an MPC control strategy.

Biography: Associate Professor Trimboli received his Ph.D. in Control Engineering from University of Oxford in 1989. He joined the faculty of the University of Colorado, Colorado Springs in 2011, where his research focuses on development of control strategies for the management of high-capacity battery systems such as found in electric vehicles. He is currently UCCS principal investigator (PI) of a multi-year program with the Office of Naval Research (ONR) headed by Utah State University where he leads a team investigating the application of model-predictive control to improve the performance and extend the lifetime of lithium ion battery cells. Other research efforts include: physics-based reduced-order modeling of ideal lithium-ion dynamics, physics-based modeling of lithium-ion degradation dynamics, empirical and physics-based modeling of lithium-ion thermal dynamics, as well as predictive methods for power estimation.
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Battery modeling and system simulation: a support for battery pack sizing and design considerations

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The battery pack system is the key component of an electrified vehicle. Its sizing, geometric and thermal design elements and its electro-thermal management considerations, have a direct impact on the pack performance, durability and safety. It is therefore required to develop design assistance tools for engineers that help to optimize the vehicle usage.

Many battery models with different levels of complexity for multiple purposes have been developed. One target is to use these developed models in system simulation software and provide assistance for battery pack sizing and design. IFPEN has been developing and enriching a set of models and tools for a dozen of years. Since 2012, these models are implemented into the Electrical Storage library of the integrated simulation platform for multi-domain mechatronic systems simulation Simcenter Amesim commercialized by Siemens PLM Software. This library holds generic and pre-calibrated electro-thermal models for common storage system’ technologies, ranging in complexity from simple quasi-static models to fine electrochemical models. These models may include aging behavior and the thermal runaway reaction of Li-ion batteries.

This work aims at presenting the abilities of these simulation tools for pack sizing and design. Different examples using simulators at various scales (from cell to vehicle) will be given to discuss sizing, lifetime, thermal management, optimization of a fast charge profile, and propagation of thermal runaway.
Model reduction for Li-ion batteries

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The pseudo-two-dimensional (P2D) model proposed by Fuller, Doyle and Newman [1] has taken a predominant role in the modelling of lithium-ion batteries. This model is developed from first principles and is accepted to give accurate predictions of the electrochemical behaviour over a wide range of input current conditions. Also, it is widely acknowledged [2] that the original P2D formulation is a solid starting point to incorporate other physical effects, especially within the context of including thermal dependency within the model. However, this model is too complex to be used in state estimation algorithms for battery system control. As discussed within [3], this is mainly due to the complex system of coupled-partial differential equations required for numerical simulation. For this reason, a number of researchers [4-8] are developing simplified derivatives of the P2D model which capture the relevant features of the physical system but are computationally more efficient and easier to parameterise.

We present a comparison between different simplified electrochemical models, obtained either using asymptotic methods or model order reduction techniques, and compare these results with simulations of the full P2D model and experimental data on commercial cells. The asymptotic methods, as presented in [7-8], allow us to systematically reduce a full P2D thermal-electrochemical model down to much simpler models (in some cases a system of three ordinary differential equations). This method has the further advantage of keeping only the phenomena that have an important role in the process and, therefore, provides insight to the experimentalists on which experiments to focus. We also discuss the limitations of the asymptotic reductions, in particular regarding the relaxation dynamics of the voltage response. Within the model reduction methods, the residue grouping method is compared with the balanced truncation method to reduce the order of a single partial model with electrolyte (SPMe). The residue grouping method can be applied either analytically (from a transcendental transfer function) or numerically (from a finite element model). Residues with similar eigenvalues are grouped together to reduce the model order.

These simplified and reduced order models are then more favourable for model-based state estimation, and optimal fast charging control. Such simplifications of the model, which are complementary techniques, will also allow more efficient data fitting methods that lead to faster and more accurate characterisations as well as the possibility of real-time implementation for control purposes.

References
Optimising lithium-ion cell design for plug-in hybrid and battery electric vehicles

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Increased driving range and enhanced fast charging capabilities are two immediate goals of transport electrification. However, these are of competing nature, demanding increased energy and power densities respectively. A trade-off by varying the number of pouch-cell layers versus electrode thickness can help in achieving application-specific design of energy or power cells. Achieving this trade-off through iterative empirical testing of multiple layer choices is expensive and often produces sub-optimal designs.

In this work, we report a modelling methodology to rapidly and inexpensively design energy-density-optimised cells for electric vehicles – supplanting traditional, empirical methods. The methodology is centred around a physics-based electrochemical model that accepts inputs from vehicle simulations, enabling battery pack engineers to maximise vehicle range. We exemplify the use of this methodology for a highly topical study: by predicting an optimum cell design to avoid lithium plating during fast charging, which is considered to be one of the most challenging criteria to meet using existing battery technology.

The results, highly relevant to battery engineers and the wider automotive industry, illustrate the potential of application-tailored cell designs, and the importance of partnerships between automotive and cell manufacturers in producing efficient energy storage solutions. Furthermore, we illustrate for a plug-in hybrid vehicle how the proposed methodology could facilitate common module design of battery packs, thereby reducing the cost of offering derivative vehicle models. Of particular importance to materials scientists, we indicate that useable cell energy density can be increased by designing electrodes with better transport properties as an alternative strategy to pursuing materials with higher capacity.

This work has been published in the Journal of Energy Storage in January 2019 and is highly relevant today. We expect that the model-based nature of the work will be of particular interest to delegates of the Battery Modelling Symposium. Accompanying the poster and publication, we provide the open-source MATLAB toolbox, BOLD (Battery Optimal Layer Design), in which the layer optimisation methodology is implemented.
Composition graded electrodes for improved dynamic and cycling performance of lithium-ion full cell batteries

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Lithium-ion full cell batteries based on LiFePO 4 cathode and Li 4 Ti 5 O 12 anode are fabricated by a layer-by-layer spray printing method 1 with a continuous through thickness gradient of active material, conductive carbon, and binder in both electrodes. Compared with full cell batteries with more usual homogeneous distribution in electrodes, but with the same average composition, both C-rate and long-term cycling performance of the battery with graded electrodes are significantly improved. The improved performance of graded electrodes is shown to derive from a lower charge transfer resistance and reduced polarization at high C-rates, which suggests a more spatially homogeneous distribution of over-potential and hindering of the side reaction-induced battery degradation during long-term cycling.

Reference
Advanced time integration methods for lithium ion battery simulation and optimization

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The porous electrode model developed by Newman and his co-workers [1] is constantly evolving due to the inclusion of novel degradation mechanisms, blend materials, non-linearities in parameters, mechanical and thermal effects, etc. which is directly translated into an increase in the computational cost of simulation. Another application of this kind of models is to improve cell design by solving optimization problems (maximizing specific energy or power, minimizing degradation, etc.) for a set of design parameters. Solving those optimization problems in a reasonable time requires efficient simulations and sophisticated techniques to avoid several high cost function evaluations.

Our work is focused on the porous electrode model efficiency and flexibility improvement by using state of the art time integration methods and a computationally efficient automatic space discretization library. Macroscale variables (Li+ concentration in the electrolyte, solid phase potential, liquid phase potential) are solved by finite element methods while microscale variables (Li+ concentration in the particles) are solved by a combination of spectral Galerkin and finite element methods. The weak formulation of the model is automatically built and discretized in space within the FEniCS [2] platform, arriving to a linearly implicit system of differential algebraic equations. The resulting system is linked with an open source adaptive time-integration library that we have developed and solved with Runge-Kutta and Rosenbrock methods [3], allowing to simulate a discharge of a lithium-ion battery in a few seconds on a personal computer. Moreover, the optimization problems are solved within the same framework using the discrete adjoint state technique [4] for the computation of the cost function gradient required by most optimization algorithms, which outperforms classical finite difference approximations when the number of design parameters increases.

In order to demonstrate model efficiency, simulations are performed for a blend electrode lithium ion battery based on a model extracted from [5]. Different time integration methods are compared for rate and cycling scenarios and the advantages of using advanced time integration methods are shown. Some design optimization problems are also solved and the efficiency of using the adjoint method is proved.

References
Multibunch model to simulate a battery heterogeneous operation at high power and low temperature

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Recently, the heterogeneous behavior of single cells have been highlighted by many experiments [1]–[3] and heterogeneous models have been developed to expand electrochemical models capabilities [4]. Heterogeneous effects are stronger when the cell overvoltage is high, that is, at high power or low temperature. With this poster, we would like to present our most recent works on modeling a LiFePO₄/graphite cell heterogeneous behavior using an equivalent circuit model (ECM).

Though ECM are often used as “black box models”, this study is based on a physical analysis in order to build a semi-physical model. The cell is considered as a set of numerous homogeneous parts connected in parallel and with different macroscopic electrochemical properties. Reasons for the macroscopic electrical properties to be heterogeneous are: manufacturing non-uniformities, distance to the current collectors, non-uniform pressure on the electrodes, local tortuosity, different particles sizes, etc. Homogeneous parts with close macroscopic properties, but not necessarily close in space, are virtually grouped because their behaviors are almost the same. We call these sets “bunches” and they can be modeled by any homogeneous electrical model. The complete cell model is made of several bunches connected in parallel whose equivalent electrical parameters are different: the so-called “multibunch model” [5].

Because we want to be able to model and characterize cells without knowing their internal electrochemical properties, we chose to model the bunches using Randles models with different equivalent electrical parameters. The heterogeneity sources listed above have been concentrated into “high frequency resistances” \( R_{HF} \) that combine many contributions to overvoltage such as the ones from the electrolyte, charge transfer, current collectors, contact resistances between particles, etc. In order to have different and consistent values for each \( R_{HF} \), they are computed thanks to a Weibull distribution law that is determined experimentally. Besides, each equivalent electrical parameter (\( R_{HF} \) and diffusion parameters) is a function of the cell current and temperature. Contrary to classical homogeneous Randles models, we also found that the multibunch model parameters does not need to be functions of the state of charge anymore, except for the open-circuit voltage. This opens interesting ways towards accelerated characterization protocols. This multibunch model predictions have been validated over a wide range of current (up to the cell maximum current) and temperature (0 °C and above) and it also brings some valuable insights into the cell internal behavior such as high local currents, SoC swings or also explain why a cell is still generating heat after the current has been stopped.

Part of this work was supported by the French National Agency for Research and Technology (ANRT). *Corresponding author: nicolas.damay@utc.fr

References
Physics based modelling of mass transport during polarization in a Li-ion battery

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Mobility of ions in the electrolyte has a great effect on the performance of Li ion batteries. It is therefore of great importance to understand the electrolyte properties that define the battery performance during operation, including the conductivity, diffusivities, and transport numbers. These electrolyte specific parameters should be included in a model, to predict its behavior during electrochemical polarization.

We present a model based on Newman’s methodology (to electrochemical reaction–diffusion) for mass transport under galvanostatic polarization in a Li|Electrolyte|Li symmetric cell. The reaction at each electrode is governed by Butler–Volmer kinetics and we used the modified form of the current-overpotential relationship. Insulating SEI layer on the bulk electrode is incorporated in the model. The polarization bias can influence the transfer of the ions, the formation of the electrical double layer, the influence of SEI formed on the surface of the electrode and growth rate of dendrite. Relation between voltage variations and plating/stripping of lithium anode is observed at different polarizations. Simulation of the concentration gradient in the Li symmetric cell is used to explain the dendrite growth in cell. This can be helpful in designing of new electrolytes for future Li-ion batteries or can also be used as a representative platform to describe the behavior of Li metal anodes.
Lithium-ion battery degradation model: estimation & prediction

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The importance of lithium-ion batteries rapidly grows each year. Sustainability trends like replacement of traditional gasoline engines with electrical powertrains gives a great boost for this process. Siemens works in this field as well. For instance, there are the fully electric aircraft Magnus eFusion and the first passenger electric ferry in the world – Ampere. Safety aspects and high costs of the aforementioned systems elucidate the need to implement battery degradation toolbox for high-fidelity life-time estimation and prediction.

Our current research primarily focuses on the topics of estimation, prediction and control of lithium-ion battery degradation. Our poster will be composed of the following contents:

- Estimation
  - Results of Kalman filter implementation for State-of-Charge and State-of-Health estimation which are based on the lithium-ion battery equivalent-circuit and physics-based models and data from the energy storage systems from the field
  - Least Squares techniques results for lithium-ion battery State-of-Health estimation for short-term and long-term ageing datasets

- Prediction
  - Fitting results overview of different empirically based degradation functions for calendar and cyclic ageing datasets

\textit{Keywords: Lithium-ion battery; Degradation}
Infrastructure networks for charging electric-vehicles through physics-based transient systems (INCEPTS platform)

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An innovative platform called INCEPTS has been developed to intelligently place chargers in a target area. By coupling vehicle dynamics and battery dynamics modeling, INCEPTS is uniquely able to accurately incorporate the impact that the environment has on the range of the battery into the placement of the chargers. This allows the INCEPTS platform to properly satisfy the charging demand of the electric vehicle (EV) fleet while also minimizing the cost needed to develop this infrastructure by maximizing the utilization of each charger. The platform utilizes a map of the target area to create a matrix representation upon which the simulated vehicles will travel on. These vehicles can be of various types such as motorcycles or cars and will each have their own randomly generated start and end locations on the map. A navigation algorithm known as A* will then route each vehicle through the map from the its respective start location to its corresponding end location. Along the way, the State of Charge (SoC) of the vehicle will be calculated and if the SoC of the vehicle gets below a set threshold, the vehicle will travel to the closest charger.

Using a high-performance computing cluster, the platform can run several simulations of thousands of vehicles in parallel, each generating their own heat map for optimal charger placement. By gathering the distributions for each charging location for a given input condition set, the convergence of the platform on a single solution can be measured. The platform was run on several different conditions including weather to compute how sensitive the demand is to various driving conditions. Comparing hot and cold weather, it can be seen that chargers tend to be placed in large population centers during hot weather seasons while the chargers tend to be placed more evenly across the map in cold weather conditions. Using the coefficient of variation (CoV) as the measurement for convergence, it was shown that under these conditions, motorcycles have an average CoV of about 14 % with a standard deviation of 6 % which increases with increasing size of the vehicle up to that of a car which had an average CoV of about 31 % with a standard deviation of 13 %. This is a result of the larger battery packs that are available to the larger vehicles.

Figure 1: Overall process for simulating the trip of an individual vehicle. The S and E icons represent the start and end locations respectively while the small dots between represent the route that has been calculated for that vehicle using the A* algorithm and their color corresponds to the traffic flow at that position.
Statistical approach to a quantitative comparison of different lifetime models for lithium-ion batteries

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The ageing of lithium cells involves multiple interdependent processes making its modelling a challenging engineering task. This work investigates ageing models \cite{1,2,3}, which rely on simple approaches, leading to a fast computation-time and a straightforward parametrization. Ageing functions with few parameters are widely discussed in literature and used in practice, while the quality of the predictions is not clear.

To get a hold on the quality of the prediction we analysed an ageing dataset regarding its statistical attributes \cite{4}. The investigated dataset is composed of 48 individuals under the same testing conditions. The statistical attributes that describe the spread of the modelled data is the covariance matrix. From the given experiment, we see that data is not homoscedastic. This means that the covariance is not constant. Therefore, we are looking for an alternative structure of the covariance by analysing the test data carefully. The goal of this publication is to present a meaningful model for that reproduces the empirical covariance structure. Further we estimate the parameters of the presented model by fitting the function to the empirical covariance matrix.

The model for the covariance structure can be used to estimate the covariance for other battery ageing tests.

\textit{Keywords: Li-ion batteries, ageing, modelling, prediction, uncertainty}

\textbf{References}
\begin{enumerate}
\item J. Schmalstieg et al., A holistic aging model for Li(NiMnCo)O\textsubscript{2} based 18650 lithium-ion batteries, Journal of Power Sources 257, 2014
\item I. Baghdadi et al., Lithium battery aging model based on Dakin's degradation approach, Journal of Power Sources 325, 2016
\item E. Sarasketa-Zabala et al., Cycle ageing analysis of a LiFePO\textsubscript{4}/graphite cell with dynamic model validations: Towards realistic lifetime predictions, Journal of Power Sources 275, 2015
\item T. Baumhöfer et al., Production caused variation in capacity aging trend and correlation to initial cell performance, J. of Power Sources 247 (2014), p.332
\end{enumerate}

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TOWARDS IMAGE BASED MODELLING OF LITHIUM-ION ELECTRODES

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INTRODUCTION

Mathematical models have been used to simulate the physical and electrochemical processes occurring inside batteries in order to aid understanding and design. Newman et al. developed one of the most popular lithium ion battery models based on the porous electrode and concentrated solution theory. Newman’s pseudo-2D (P2D) model assumes that the porous electrode is made of equally sized, isotropic, homogenous spherical particles. It has been shown that battery electrodes are actually very heterogeneous structures [1] and therefore more complex approaches are required in order to fully characterise the transport processes occurring within the battery.

This work develops a data-driven, image-based modelling framework that is capable of modelling lithium-ion battery electrodes.

METHODOLOGY

A number of different imaging techniques are capable of providing electrode data, namely: scanning electron microscopy (SEM), focussed ion beam scanning (FIB) and x-ray computed tomography (CT). SEM techniques reach suitable resolutions (~0.5 nm) however they only provide 2D data, therefore they cannot capture the full 3D volume of the electrode. FIB scanning uses a beam of positively charged ions to null away the surface of the target and so is a destructive method, therefore in-situ testing or re-testing of a battery would not be possible. State of the art CT scanners can achieve sub-micron resolutions whilst being a non-destructive method, for these reasons CT imaging was chosen.

Finite element based models have been used extensively to simulate lithium-ion batteries [2] however they have been shown to be computationally expensive to mesh the image data. Finite difference schemes use a regularly discretised mesh and are usually quicker to implement, as the voxel dataset can be used directly, but they can result in approximation errors. Adaptive mesh refinement (AMR) is a technique used in finite difference schemes to refine or coarsen the grid around regions of sensitivity, both spatially and temporally. An example of block-structured mesh refinement can be seen in figure 1, this is a technique that allows for quick implementation of the mesh whilst retaining accuracy.

RESULTS AND DISCUSSION

The first electrode to be imaged was an uncycled titanium dioxide sample on a carbon polymer substrate, originally made for an aluminium ion battery. The titanium dioxide layer is approximately 20 µm thick, meaning it is a thinner film electrode than the equivalent lithium-ion graphite, allowing the full capabilities of the CT equipment to be tested. The scan was carried out with a 20x magnification lens and a voxel size of 481 nm; the total scan time was 16 hours. An individual tomographic slice can be seen in figure 2.

![Figure 2: Individual tomographic slice of a TiO2 layer on a carbon polymer substrate, voxel size 481 nm.](image)

The CT dataset is then post-processed, using an anisotropic diffusion filter to reduce the noise/distortion from the scan. The dataset can then be thresholded into appropriate phases, in this case fluid and solid as seen in figure 3. This dataset can then be used as the computational domain for subsequent physics calculations.

![Figure 3: Thresholded electrode data set, voxel size 481 nm.](image)

CONCLUSIONS AND FUTURE WORK

This work has started development of a single-physics, image-driven computational model. An imaging method has been established to obtain electrode microstructural detail and initial results have been shown. Work is ongoing to carry out physical simulations on imaged electrode datasets. The final goal will be to fully expand the model to multi-physics simulations.

REFERENCES

Modelling the electrochemomechanics of solid electrolytes

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Solid-state lithium batteries cannot be made to cycle at reasonable power because of dendrites, whose formation mechanism remains uncertain. The critical current above which dendrites nucleate in lithium-conductive ceramic electrolytes is elucidated by a theory considering the mechanical consequences of electrochemical phenomena [1] such as space charging and charge-transfer reactions. Applied voltage can induce stress in solid electrolytes; dendrites are found to nucleate in polycrystalline Li$_7$La$_3$Zr$_2$O$_{12}$ (LLZO) garnet [2] when the interfacial pressure reaches a critical value. This critical pressure can be related to the surface-energy change incurred by lithium plating in grain boundaries. A derived formula, quantitatively validated with experimental data [3], predicts how critical current depends on properties including interfacial impedance, bulk permittivity, and grain size. As well as suggesting strategies by which materials can be designed to suppress failure, the proposed mechanism rationalizes the electrically activated transition from stable low-current cycling [4, 5] to fracture-driven dendrite propagation [6] above the critical current. The impedance model of LLZO leads to a physically justified equivalent circuit of LLZO between two blocking electrodes (e.g., Ni). Bode plots show a signature of space-charge layers, which can be used to measure the charge carrier concentration in LLZO.

References
Electrical energy storage management for low carbon grids

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Grid-connected battery energy storage systems (GBESS) are a key technology for power network stabilization and other auxiliary services, as the penetration of renewable generation increased. However, while the price/capacity/life trilemma of batteries still exists, a deep understanding of the batteries characteristics and system architecture needs to be established for control method study to exploit the best performance of the whole GBESS.

Up to the presented stage of research, different battery models in literature were reviewed and laboratory tests were done for the lithium-ion battery used on a commercial GBESS called SIESTORAGE to obtain parameters for suitable battery models and to evaluate characteristics. For example, a round-trip energy efficiency of 94% was observed in battery tests. Second, the battery performance obtained was related to the SIESTORAGE system operation and in the efficiency analysis and the battery contribute half of the total round-trip loss of the system, which was presented at IET PEMD Conference, 2018. Third, control strategies were studied and implemented in MATLAB for using the GBESS in price arbitrage scenario to optimise the profit with consideration of battery degradation. An optimisation model was built with electricity price as the input, battery operational power as the output, and battery state of charge and capacity degradation as state variables.
Demystifying Li insertion in graphite via reduced order models: validation by measurements of OCV and entropy change

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Achieving predictability in the performance and degradation of lithium-ion batteries requires unifying the current scales gap between atomistic and continuum models, needing physically informed and experimentally validated parameters for the open circuit voltage (OCV), E_{OCV} and its derivative with respect to temperature dE_{OCV}/dT. The latter, related to configurational entropy of Li/vacancy arrangements in the electrode materials [1-3], is proportional to the reversible heat generated during charge and discharge.

Here, we utilise a modified two-level Bragg-Williams approach [3,4], allowing fast comparisons between experiments and models of OCV and entropy with minimal input parameters. We can thus describe features known from Li/graphite phase diagrams, such as order/disorder transitions, previously determined from in-situ neutron diffraction measurements [5] and first principles models [6]. These features, usually missing from empirical models of Li intercalation, should be included in a proper description of the entropy coefficients. Via a similar approach, we successfully modelled order/disorder transitions in lithium manganese oxide spinel with systematically varied point defects and validated the model with experimental data [3,7]. Here we model the OCV and entropy change of the Stage I – Stage II transition in graphite [4,6,8], also approximating the transitions that occur at low lithium occupation. We validate the model through direct measurement of the entropy change and OCV during charge and discharge at different temperatures. Both measurement sets show an apparent hysteresis effect [9].

Through our models, and measurements conducted at variable temperature, we propose the possible structural and phase change origins of this effect. Hence we provide rational explanations as to how and why the observed features change in position and amplitude as a function of temperature.

References
The poster deals with physics-based ageing modelling being developed in a shared project between Oxford University and VITO – EnergyVille (Genk, Belgium). Open access software is developed in which many the various models from literature are implemented for ageing effects such as SEI growth, loss of active material and surface cracks. This software has been applied on test results from cells in the Eco Com’Bat project under the EIT RawMaterials consortium.

To enable sufficient data for separating ageing effects, a test regime consisting of calendar life tests and cycle life tests is necessary. This is different from using driving cycles to age cells. Such a programme has been set-up within the H2020 project Everlasting. The test scheme will be shown. Since the reaction rates of ageing effects appear to be highly temperature dependent, tests at several temperatures are necessary. The cell heating during cycle life tests have to be considered in fitting parameters.

The test set-up has been explained in: “White Paper on Test methods for improved battery cell understanding”. This document can be found at: https://www.batterystandards.info/ under the section ‘Literature’.
A pseudo-2D model for lithium plating/stripping of graphite electrodes that includes chemical intercalation

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In 1999, the pseudo-2D model [1] of lithium-ion batteries was extended by Arora et al. [2] to include lithium plating and stripping at the graphite-based negative electrode. Arora et al.’s model has since been further developed to include effects such as temperature dependence, [3] porosity change and SEI growth [4]. However, no models of chemical intercalation, where plated lithium intercalates into graphite without generating a current, exist at present. If chemical intercalation is ignored, both in-situ and destructive methods of plating detection could underestimate how much lithium was plated. [5]

In this work, Arora et al.’s lithium plating/stripping model is combined with the porosity reduction model of Sikha et al. [6] and a new equation for chemical intercalation. The resulting three-process model, illustrated in Figure 1, is implemented in COMSOL and compared with charge/discharge cycle measurements at 273 K, which include CCCV charging at up to 5 C.

References
A nonlinear model predictive control approach for the balancing-aware charging of series-connected lithium-ion cells

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In the last decades, the ever-increasing demand for portable devices as well as hybrid and electric vehicles has pushed the development of high performance energy accumulators. Among them, Lithium-ion batteries currently exhibit the most remarkable performance in terms of energy and power density, efficiency and low self-discharge. In order to match the requirements of the different applications (in terms of e.g. power, driving range, etc.), battery packs are usually composed of dozens of cells which are arranged in series and parallel connections. Due to unavoidable inconsistencies, both in the manufacturing process and in the operating conditions, the cells composing a battery pack exhibit slightly different features which lead to charge unbalance over time if conventional charging methods are used.

In this work, a general nonlinear MPC formulation for balancing-aware optimal charging of series-connected lithium-ion cells is proposed. In particular, we aim at finding the optimal input current which should be applied to each cell in order to guarantee fast charging and state of charge balancing at the end of the charge, while satisfying safety constraints. An ad-hoc electrochemical model is developed to be employed in the proposed algorithm. The concepts are subsequently specialized for an easily implementable power supply scheme, in view of the possibility of a practical implementation. Finally, the proposed approach is validated on commercial cells using the Lithium ION SIMulation BAttery (LIONSIMBA) toolbox.

The results highlight the effectiveness of the proposed method when compared with standard charging strategies, both in terms of battery exploitation and safety. Moreover, due to the fact that using the presented approach the balancing goal is directly considered during the charge, the need for an offline balancing protocol is completely avoided.

This work has been submitted to the IEEE Transactions on Control Systems Technology.
Experimental validation of a physical energy management system to increase revenue and lifetime of grid-connected Li-ion batteries

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The increasing deployment of renewable energy sources opens up new opportunities for grid-connected energy storage. Lithium-ion batteries offer extra flexibility compared with most other storage technologies. The techno-economic assessment of the investment, and the energy management system (EMS) controlling the battery, typically use simplistic battery models. Recent research has shown the theoretical possibility for increased profit and lifetime using more realistic battery models in the economic optimisation \cite{1}. Although promising, the conclusions were all based on simulations.

Therefore, experiments were conducted to validate those findings. One of the profiles tested represents how grid-connected batteries are used today: the battery is only allowed to cycle in the middle 80\% of its full state-of-charge window to avoid excessive degradation and over- or undercharge, and the battery is only used if the revenue exceeds a given threshold. Another profile represents revenue maximisation, but without consideration of battery lifetime. Finally, the profile from the advanced control, which used a physical battery model, was tested. Each profile was tested on two cells using a battery tester which cycles the cell according to each predefined current sequence.

The figure opposite shows the cumulative revenue and degradation cost for each cell. The results labelled ‘SPM’ from the advanced control; the results labelled ‘BM\textsubscript{P}’ are from the conventional control; the results labelled ‘BM\textsubscript{R}’ are from the revenue maximising control. Even though the test has only been running for 2000 hours, we can already observe that the advanced controller can simultaneously increase the revenue (+11\%) and decrease the degradation cost (-15\%) compared to the conventional control. Ignoring the degradation cost results in a suboptimal outcome where although the revenue can be increased significantly, due to the higher utilisation the degradation cost increases much more.

Finally, the implications for grid-connected batteries are discussed. In order to use this advanced control, a closer integration between the EMS (which determines battery charge/discharge setpoints) and the BMS (which controls the battery to follow the load profile) is needed. A real-life setup has been developed where a small battery module is connected to an on-board BMS system, a battery tester and a computer with the EMS. The goal is to find out how this integration can be practically achieved, and if the results from the previous experiment translate well to a real-life battery.

Electrochemical models for fast charging algorithms in battery management systems

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As one of the most critical factors for a widespread adoption of electric vehicles, fast charging capability of lithium-ion batteries has evoked increasing research interest [1]. The charging current and therefore the charging time is mainly limited by the battery temperature as well as the danger of lithium plating on the anode [2]. While the battery temperature can be measured by means of temperature sensors, the anode potential, which is the main indicator for lithium plating, cannot be easily observed without an integrated reference electrode. Electrochemical models implemented in the battery management system improve fast charging algorithms especially for low temperatures by estimating the anode potential [3].

However, due to inevitable inaccuracies in the modelled effects and model parameterization, the predicted behaviour of the battery cell will diverge from a real battery cell over time. This motivates the use of state estimation techniques like Kalman Filters to correct model states with respect to physically measurable quantities i.e. current, temperature and cell voltage [4]. These approaches are mostly combined with model simplification techniques such as polynomial diffusion profiles, orthogonal collocation techniques or single particle models [5]. Many simplifications decrease the accuracy of model predictions of the battery behavior, especially at high charge and discharge rates as well as dynamic load profiles [6], limiting the applicability for fast charging control. In addition to that, most existing estimators are solely designed for correctly reproducing the full cell voltage, which does not necessarily result in estimates of the anode potential that ensure a safe control of charging currents.

In our poster, we will present different Unscented Kalman Filter (UKF) estimation strategies employed with a full-scale, flexible C++ implementation of the Doyle-Fuller-Newman (DFN) model based on [7]. This allows the optimized fast charging of a lithium-ion battery by anode potential estimation. Special emphasis is put on ensuring a conservative anode potential estimation to decrease the likelihood of lithium plating. This is approached by favoring model corrections which lower the estimated anode potential while charging. The model filter combinations are tested using a finer discretized model with realistic measurement noise-affected output values as a simulated measurement input. Our results are evaluated with respect to both the output voltage as well as anode potential accuracy at different model scales and distortions where predictions of anode potential do not exceed simulated real anode potential.

References
Machine learning for the diagnosis of battery state of health from impedance spectra

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The possibility of diagnosing Li-ion battery’s state of health (SoH) and remaining useful life from electrochemical impedance spectra (EIS) using Machine Learning is investigated. The Gaussian Process (GP) with automatic relevance determination is used to identify degradation patterns without relying on any equivalent circuit models. The experiment consists of continuous charge-discharge cycling of commercial Li-ion coin cells. With the GP model trained with the entire spectrum measured on identical cells cycled under the same condition, the cycle number of a testing cell can be predicted by providing the corresponding EIS data. Moreover, the trained GP model selected one frequency that shows the most relevant feature to the battery degradation, indicating the potential that battery SoH can be diagnosed by measuring impedance at certain frequency component(s) instead of taking a full-range EIS. By extracting the change of the spectrum with cycle numbers at that frequency, we identify the degradation pattern of coin cells by revealing a close relationship between the growth of charge transfer resistance and the degree of fading.

Multi-Dimensional Modeling and Simulation of a 18650 nickel-rich, silicon-graphite lithium-ion cell for developing rapid charging methods


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Increasing the energy density of lithium-ion batteries recently favoured the usage of highly densified electrodes at low porosities (< 20 %) and high-capacity active materials such as nickel-rich cathodes and graphite anodes including small amounts of silicon. As seen in our experimental tests of such a 18650 high energy cell (INR18650-MJ1, LGChem), safety issues in form of critical overheating during rapid charging (> 65 °C for C-rates > 2C) and accelerated cyclic aging appear (< 200 cycles for SoH < 80 % at 1C), which may narrow the application area and lifetime of the cell. Therefore, internal battery states such as concentrations and potentials in the electrolyte and the active materials can be simulated not only over the thickness of the electrode stack, but also along the electrodes to avoid critical and harmful states and maintain safe operation and prolong the overall lifetime of the battery. We present a multi-dimensional, electrochemical-thermal cell domain model [2] incorporating several parallel-connected pseudo-two dimensional (p2D) models [1], a single 2D electrical model and a 3D thermal model. The submodels are used to simulate local potentials and concentrations in the electrode stack (i.e. anode, separator and cathode), polarization effects on the current collector foils and local heat generation as well as temperature distribution in the spirally wound jelly roll, respectively. The model is used to study different electrode designs in form of different tab patterns for the 18650 cell and its influence on the inhomogeneity of local current density and temperature distribution. It is shown, that optimized, multi-stage constant current rapid charging profiles based on the local, simulated anode overpotential and local cell temperature can be simulated in dependency of the electrode design to avoid harmful lithium-plating.

The parameterization of the model includes open-circuit potential (OCP) measurements of the full-(INR18650-MJ1) and custom-built half-cells (Ø 14 mm) [2]. Electrode properties are defined via laser microscopy, mercury porosimetry, inductively coupled plasma-optical emission spectroscopy (ICP-OES) and weight measurements [6]. Accelerating rate calorimetry (ARC) and infrared thermography measurements under convective cooling conditions (vair=1 m s⁻¹) are applied on the INR18650-MJ1 to validate the parameterization [6] and estimate the error of the simulation results. Figure 1 illustrates the implementation of the multi-dimensional model incorporating the three submodels implemented in the FEM-solver COMSOL Multiphysics 5.3a and the simulation results for evaluating the electrode designs towards their capability of rapid charging methods.

![Graphical abstract](image)

Figure 1 Graphical abstract.

References:

An asymptotic framework for battery modelling

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Mathematical modelling of batteries provides a mechanism to manage them efficiently and maximise their lifetime. The two main modelling approaches are full physical models and equivalent-circuit models. The former are computationally expensive to solve, while the latter do not provide physical insight. Our aim is to develop simplified models, based on the physical models, which provide the same insight but can be solved more efficiently and hence used for live battery management, on-line diagnostics, and cell design.

Starting with a full three-dimensional dynamic model with concentrated electrolyte theory, we use asymptotic analysis to systematically derive simplified physics-based models. The asymptotic limits taken can be roughly categorised into those that result in simplifications at the macroscale or the microscale. At the macroscale, we exploit the extremes of cell aspect ratio, electrode conductivity and electrolyte diffusion. At the microscale, we idealise to a distribution of spherical particles, and then take limits in which this distribution is narrow and diffusion in the particles is fast.

These limits create a matrix of possible models. We present the general framework for this matrix, as well as results for four groups of models. Firstly, in the limit of small aspect ratio, we present temperature and potential distributions in the current collectors and decompose the voltage into its constituent overpotentials. Secondly, our framework allows us to systematically produce, in the limit of fast electrolyte diffusion, a more accurate version of the single-particle model with electrolyte (SPMe), which we compare to existing results. Thirdly, we consider a distribution of particle sizes and present a corrected single-particle model in the limit that the distribution is narrow, i.e., the variance is small. Finally, we consider the limit in which diffusion is fast in particles (lithium iron phosphate), or there is no intercalation (lead-acid), and investigate how well the behaviour is described by models of different fidelity.

The approach provides a general framework for developing reduced-order models that can be applied to many chemistries, and extended to incorporate additional physical effects such as mechanics, side reactions, and degradation mechanisms. Additionally, we are currently developing the software package PyBaMM to implement the suite of models numerically.
Theory of local fluctuations of ion concentration and potential in porous electrodes

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Newman and coworkers have developed an electrochemical model of battery with porous electrodes that allows to predict many characteristics of charge-discharge cycle (voltage, potentials in different phases, etc.) quite accurately [1,2]. The model is computationally effective because it generally neglects the spatial microstructure details, substituting them with averaged or representative features instead.

Newman’s model can be derived through application of averaging procedure to the microscopic transport equations that govern the processes in the electrode phases [3]. The applicability of the averaging can be justified within the mathematical framework of homogenization theory [4] or with numerical experiments, in which one compares running averages with the predictions of Newman’s model [5].

There are, however, processes (degradation, including SEI formation, lithium plating, heat generation, etc.) whose proper description requires tracing the local fluctuations of physical quantities on the microscopic level. These fluctuations are averaged out in Newman’s model. One can extract the relevant information from a microscopic numerical simulation, but it is much more computationally demanding. A systematic theoretical understanding of the connection between the fluctuations and the microstructure geometry is missing as well.

To bridge this gap in the theory, we are developing an extension of Newman's model that predicts the local fluctuations of ion concentration and potential by combining insights from numerical simulations with mathematical analysis. We will present results on the dependence of the overpotential fluctuations on the shape of active material particles. Our ultimate goal is to produce a model that treats the fluctuations in a statistical manner and requires less computational recourses than the exact microscale model of [5].

References
5. A. Latz, J. Zausch Beilstein J. of nanotechnology 2015, 6, 987-1007
Tracking the capacity fade of Li-ion batteries using an Ampere-hour model and entropy profiles

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The electric vehicle industry has known a rapid development in the recent years. Indeed, increasing concerns regarding global warming, such as CO2 emissions, led automakers to implement cleaner technologies in their vehicles. For instance, to be competitive with thermal engine vehicles, a lot of work is carried out to enhance the energy storage systems of the electric vehicles (EV) in order to improve their autonomy and performance.

Thus, it is essential for automakers to understand how driving conditions affect the battery ageing as it results in capacity and power fade. These parameters estimation can be made by using different approaches, from detailed electrochemical equations to mathematical data-based models. Yet, none has so far performed enough to obtain a real time battery ageing estimation in EV application. In this work, a semi-empirical approach is presented and aims to model the ageing of LIB’s. To begin with, the Ampere-hour approach consists in adding the constraints related to the cycling conditions in order to determine a capacity loss \[1\]. More in details, several weighting functions are defined for each cycling parameter, such as the applied current, the cycling temperature or the elapsed time. Consequently, it is possible to quantify their relative impact on the capacity loss. Therefore, by summing all the constraints related to the cycling of the battery, an estimation of the state of health is made.

Secondly, the entropy profiles of the batteries are measured \[2\] throughout their ageing. These will be analyzed to understand the underlying ageing mechanisms of the batteries and to find a deeper correlation with their states of health. For instance, identical batteries were cycled at room temperature using different charging and discharging current rates. The obtained results have shown linear relationships between entropy coefficients evolution at low-SOC and the capacity loss of the battery for all the tests. On the other hand, charging and discharging cycling conditions have contrasting impacts on the entropy profiles at lower states of charge. Complementary experiments at different temperatures and current rates will be carried on in order to enhance the presented approach. The robustness of this model relies on the mixing of several parameters (capacity and entropy profiles) to estimate the battery ageing. Moreover, it will allow us to optimize the EV life of the battery throughout a good knowledge of the cycling conditions impact on its ageing.

References

A multiphysics model based on LS-DYNA platform

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With the increasing number of electric vehicles, inevitable accidents, vibration and foreign object penetration potentially generate catastrophic consequences such as fire or explosion. Unlike traditional engineering materials or structures, lithium-ion batteries (LIBs) exhibit multiphysical behaviors including mechanical deformation/failure, thermal conduction, and a series of electrochemical and chemical reactions, upon mechanical abusive loading. Therefore, developing computational frameworks capable of describing multiphysical behaviors of cylindrical batteries in crash safety design of electric vehicles based on commercially available platforms is in pressing need.

In this poster, based on the widely used LS-DYNA software platform, a multiphysics model with the comprehensive coupling of mechanical, battery, short-circuit, exothermic and thermal models are established. Models are validated by the in-house designed experiments. Further, parametric studies based on the established model demonstrates that a larger indenter leads to a later onset of internal short circuit for LIBs but result in a higher peak battery temperature. This study provides an accessible, fast and accurate computational framework for safety design, assessment and improvement of lithium-ion batteries and electric vehicles in harsh mechanical scenarios.