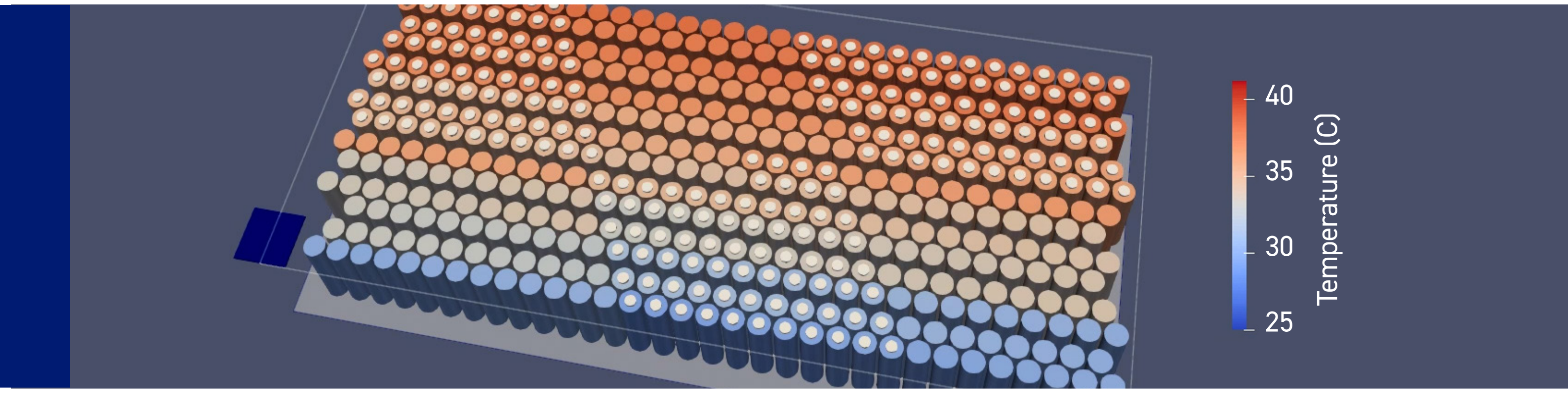
Faraday Insights - Issue 15: December 2022
Institute for Molecular Science and Engineering Briefing Paper No. 8

The Value of Modelling for Battery Development and Use



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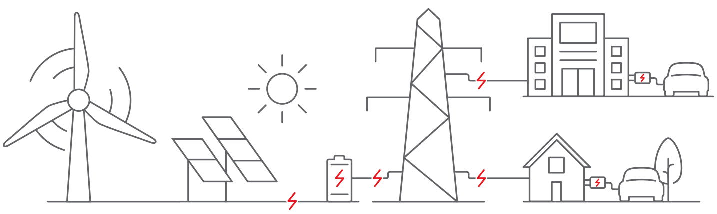
Batteries are important enablers of clean energy and mobility, but improvements in performance, longevity, safety and sustainability are needed. Battery models used to design a product on a computer save time and reduce the number of expensive physical prototypes needed. Computer models at multiple scales consider not only the properties of materials, components and cells, but also the impacts on pack functionality and across the lifecycle. Model simulations are often the only practical way to predict battery performance or battery failure, ensuring their safe and efficient operation.

Introduction

Energy storage, in the form of batteries, is an important enabling technology for supporting the transition of the UK to a green economy.[1] The high power, energy density and rapid response times of batteries provide power for electric vehicles (EVs), as well as much-needed flexibility for buffering the intermittency of renewable energy sources in domestic and grid installations.

Figure 1: The role of batteries within the electricity and transport systems



Battery models lead to better batteries

Developing a new battery pack with a predefined and well understood operational performance (i.e., rate of battery degradation, temperature performance and control) requires detailed performance metrics across multiple scales (operational, pack, battery management system (BMS), module, cell, and materials levels).

Models that consider different avenues for improving batteries, at all scales, and the trade-offs between them, are very powerful tools, enabling industry to make rapid advancements in battery performance and select the most profitable or cost-effective option.

These metrics could be obtained through considerable numbers of prototyping trials and from experimental data generated over long periods of development. However, this approach is highly resource intensive and is unsustainable for new market entrants and companies specialising in small volume / high value custom products. As such, reducing the number of experimental trials to accelerate battery development will be of clear benefit to numerous UK companies.

Computer modelling is a powerful tool that helps industry to:

- Reduce the time and cost for developing new batteries;
- Increase the understanding of how new materials impact

Image: Simulation of heat generation during discharge across an entire electric vehicle battery pack using DandeLiion
[1] The Ten Point Plan for a Green Industrial Revolution

cell performance; and

- Improve battery management systems, thereby reducing warranty costs.

In short, models help researchers to deal with complexity and keep track of all the dynamic interactions between all components. Computer models can be used as digital prototyping tools for designing battery cells and packs rapidly and safely, avoiding the time and cost required to physically construct each design. Models can also pinpoint the limitations of a new design or illustrate how temperature impacts performance. They may also be used to predict lifetimes, calculate return on investment, or estimate how much charge the battery is currently holding (the "state of charge") or how much charge it can supply instantaneously (the "power capability"), all of which are difficult to measure directly.

Computer models already exist for battery systems and components at various scales, but the most sophisticated tools are often highly proprietary and not easily accessed by small and medium-sized enterprises (SMEs) that are seeking to develop more niche products. Furthermore, the previous generation of available models were still severely limited in performance; improvements in speed, accuracy and usability are still desired. As such, there is demand from industry for well-parameterised computationally low-cost models that are both fast and accurate.

The Faraday Institution's Multiscale Modelling project[2] is focused on advancing the modelling of lithium-ion batteries to meet these challenges. This includes driving the development of modelling standards to reduce the risk of market fragmentation and in support of reduced costs, scale and agility.

This Insight will outline the role modelling plays in the development of batteries, including battery chemistries

Box 1: What are computer models?

A computer model is a digital representation of a real-world system, where the mathematical interactions between components are defined in accordance with scientific theory. Scientists make extensive use of computer models to help understand the processes and phenomena that govern behaviour in many complex systems.

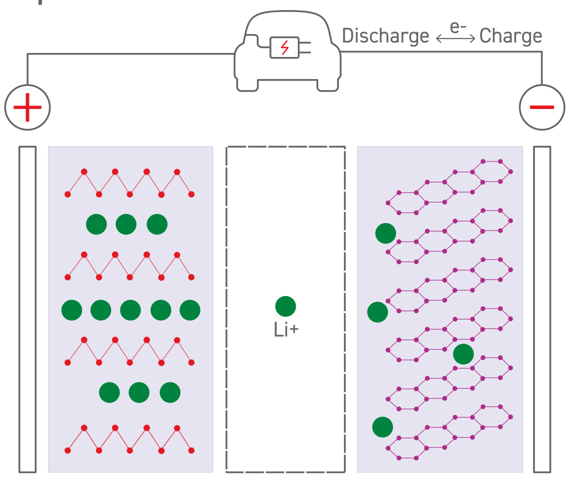
Models are valuable for researchers to identify efficiently the dominant factors, design optimal structures, maximise operating conditions and develop control mechanisms to satisfy the needs of certain applications. The answers to questions like "how much will it cost to deploy batteries widely in the transport sector", "how sustainable is a new battery chemistry" or "will this new type of battery be safe to run in extreme temperatures" are not straightforward but are determined by many interdependencies between parameters.

that are currently commercialised, as well as future developments in battery technology (short and long-term).

Battery models need to capture the complexity of the battery system

Batteries store electrical energy as chemical energy and release it as electricity when needed. Lithium-ion batteries consist of a series of electrochemical cells, each with two electrodes, positive and negative, immersed in an electrolyte with a porous separator in between, electrically insulating the two electrodes from each other. During discharge, electrochemical reactions at the negative electrode (the anode) separate an electron from each lithium atom, leaving a positively charged lithium ion. Metal sheets in contact with the electrodes allow the electrons to flow through an external circuit, generating electrical power. The lithium ions migrate through the electrolyte and across the separator to reach the positive electrode (the cathode). During charge, the reverse process occurs, and lithium ions and electrons are driven back to the anode by the charging current. In order to provide the power and energy an EV or grid-storage battery needs, battery packs combine a large number of battery cells together into one device.

Figure 2: The internal structure of a lithium-ion battery and how it operates



At the smallest scale, to gain a fundamental understanding of how the ions move and what barriers they face, models need to simulate the interactions between the atoms and molecules for each of the materials within the battery. To see how this impacts the functioning of the cell, models need to encompass all the constituent components and simulate the whole cell. Insights into how these cells interact together and what may limit their functioning also requires a simulation of the entire battery pack.

The economic value of battery modelling

Improved battery modelling could substantially benefit the UK economy by helping SMEs develop batteries and EVs for specialist and high-value markets, as well as offering warranty

[2] Multiscale Modelling Project website.

providers with more accurate performance predictions. Most EV battery warranties have several different features, typically a 5 to 8-year warranty, a 100,000-mile limit[3] and/or a 30% loss in capacity. To manage warranty costs, original equipment manufacturers (OEMs) need to understand the type and frequency of faults in EVs, whether arising from driver behaviour, fundamental design limitations or degradation of the underlying battery materials. Computer modelling is therefore increasingly used to develop and improve battery management systems, providing:[4]

- increased battery safety and longevity;
- accurate state-of-function, state-of-charge and state-of-health data;
- reliable prompting for caution or indication of a need for a service investigation; and
- signalling of the end-of-life when the capacity falls below the user-set target threshold.

Box 2: BMS and auto warranty market

The size of the BMS market and the amount of expenditure on warranties provides an indication of the markets that battery modelling addresses. The global BMS market size is estimated to reach £12 billion by 2030[5] while the EV battery warranty market in the UK is expected to reach £0.8 billion by 2030.[6] Other revenues may also be leveraged from other parts of the battery value chain, such as lower operating costs for dealers or higher initial EV purchase price due to greater safety and reliability.[7]

The case for standardised battery modelling

Outside academia, the development of modelling methodologies to date has tended to take place in "silos" – informed by the requirements and knowledge bases associated with specific sectors and companies. Given the global importance of lithium-ion batteries as key enablers of low-carbon economies, this approach is no longer sufficient.

At a time when the design of battery-based systems needs to evolve at pace, proprietary approaches to modelling and simulation are encouraging fragmentation, overloading scarce modelling skills, impeding interoperability and inhibiting scale, all of which adds cost and increases time to market. The Faraday Institution is therefore working with industry and policy makers to develop modelling standards that aim to:

- encourage and support the adoption of advanced modelling technologies, without the costs associated with individual firms "reinventing the wheel";
- support more agile workflows;
- improve supply chain diversity by providing affordable access to world-class modelling and simulation tools to firms of all sizes – especially valuable to the UK's advanced engineering consulting & design and battery component developers.

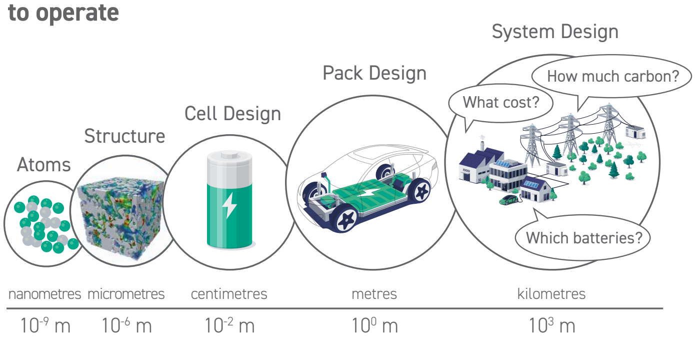
Standardisation is in no way synonymous with one-size-fits-all development. As with all standards, company- and model-specific innovation would sit on top of a standardised battery model, with more precise outcomes enabling better informed requirements to battery manufacturers.

Different Scales of Battery Models

Battery systems are complex devices containing many components manufactured from a range of materials. For models to be useful in assessing battery performance and in informing new battery designs and applications, they need to reflect the complexity of the battery itself. There are therefore many levels or scales that need to be modelled, such as simulating the behaviour of constituent materials and components, investigating how the materials work together in a complete cell and assessing how the many cells in a pack interact.

Some examples of different types of models by scale include: (1) atomistic (2) structural (3) cell design (4) pack design and (5) system design models (see Figure 3). The estimates from detailed models can be used to define models at the next scale up, forming an information pipeline.

Figure 3: The various scales at which battery models need to operate



(1) Atoms

Atomistic models for materials and interfaces form the foundation of a multiscale modelling pipeline (see Figure 3) and are key to understanding why batteries degrade and which conditions accelerate the process. Atomistic models help to develop the understanding of behaviour at a fundamental level (i.e., the interactions between the atoms and molecules) to improve the performance, safety and operational lifetime of a battery. Using known physical and chemical principles, atomistic models can estimate key material properties, such as how fast particles move, how well they perform under a range of conditions and how

3 EDF Energy website.
4 Battery management systems.
5 2030 estimate based on Research and Markets, Automotive battery management system market - growth, trends, COVID-19 impact, and forecasts (2022 - 2027).
6 Faraday Institution estimates based on projections of the size of the UK's EV battery market and a bottom-up assessment of the components of cell manufacturing costs.
7 Intellinet, Why OEMs and dealers need advanced battery warranty software? 2018.

quickly they transmit the charged particles generating the current. The high predictive accuracy of atomistic models has been demonstrated by theoretical predictions of new behaviour before it was confirmed through experiments. The presence of additional diffusion mechanisms for lithium in graphite, for example, were first predicted using molecular dynamics and later confirmed experimentally using X-ray diffraction.[8]

(2) Structure

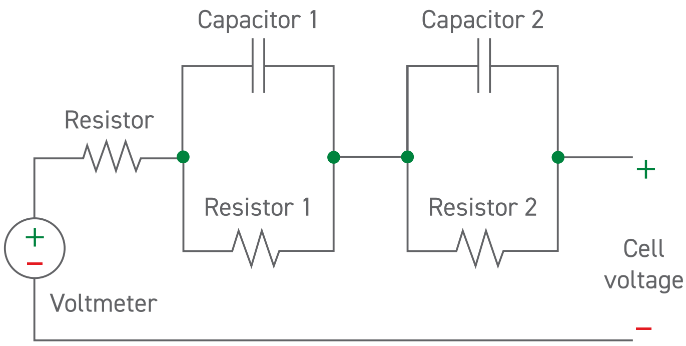
'Higher scale' models of structures reduce computation time by employing simplifying assumptions. These sacrifice some accuracy, but as long as the right assumptions are made, a high level of accuracy is still maintained. The case study in Box 3 shows how the compromise between accuracy and speed is reached for larger length scale simulations in the context of a model developed to understand behaviour at interfaces between materials. This is an important and challenging area of research that the Faraday Institution's Multiscale Modelling project is working to address.

(3) Cell design

The modelling of batteries necessitates the simulation of highly complex and interactive systems. At longer length scales, there are two approaches to modelling whole cells:

1. Equivalent circuit models (ECMs) are simulated electrical circuits containing variable resistors, capacitors and voltage sources that are designed to mimic the operation of a real electrochemical cell. The most commonly used ECM in the battery industry is shown in Figure 5, having two resistor-capacitor pairs. The parameters (open circuit voltage, resistances and capacitances) are each a function of temperature, state of charge and state of health, and are extracted from experimental voltage data. Curve fitting algorithms are used to find the optimal values for each parameter, such that the ECM voltage response to a given drive cycle fits well with the experimental data. ECMs can be easily thermally coupled, meaning predictions can be made regarding heat generation and temperature rise.

Figure 5: A typical equivalent circuit model to represent the behaviour of a battery



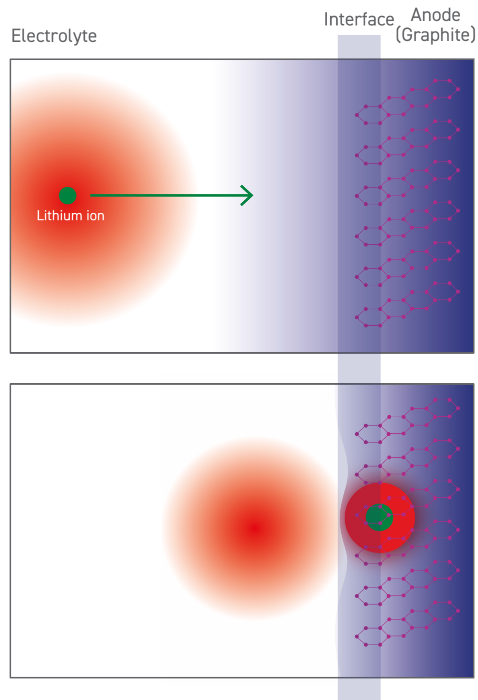
Box 3: Bringing atomistic accuracy to larger systems

Batteries are complex devices containing a range of different materials, working together. Most of the processes that could limit a battery's performance occur at the interfaces between these different materials but, to simulate this accurately, a large number of atoms would need to be included in the model. In particular, the model would need to include enough atoms from each material, the layers of atoms that come into contact at the interface and how they behave as the materials interact.

Fully capturing these dynamics increases the complexity of the model and the number of calculations required, considerably slowing down the time taken for model runs. However, the Order-N Electronic Total Energy Package (ONETEP)[9] is able to simulate interactions between a large number of atoms in a matter of hours, instead of months.[10] As part of the Faraday Institution's Multiscale Modelling project, Professor Chris Skylaris of the University of Southampton is extending the ONETEP code to be able to simulate more complex electrochemical processes in batteries.

In Figure 4, the simulation includes large numbers of atoms, representing the two materials on either side of the interface and the interactions at the contact point. The model allows researchers to investigate how easily ions move in and out of the electrode materials, which directly impacts their power output.[11]

Figure 4: ONETEP simulation of ion transport across an interface



[8] See Journal of Materials Chemistry (Issue 16. 2012), Structural requirements for fast lithium-ion migration; and Journal of Physical Chemistry Chemical Physics (Issue 28, 2013), Single-crystal X-ray structure analysis of the superionic conductor.
[9] ONETEP: linear-scaling density-functional theory with plane waves.
[10] A Bhandari et al, Electronic structure calculations in electrolyte solutions: Methods for neutralization of extended charged interfaces, J. Chem. Phys. 153, 124101 (2020).
[11] J Dziedzic et al, Practical approach to large-scale electronic structure calculations in electrolyte solutions via continuum-embedded linear-scaling density functional theory, J. Phys. Chem. C 2020, 124, 14, 7860–7872.

ECMs are not parameterised from fundamental physical properties, as with physics-based models. As a result, they should not be used for predictive modelling, where extrapolation beyond the parameterised range is required. This makes them less effective (and reliable) for lifetime and degradation modelling, and better suited to observing how a certain cell will behave under predefined operational conditions.

2. Physics-based models use mathematical equations that are known to represent the underlying physics. Historically these models have been much slower than empirical models, but there are mathematically rigorous ways to further simplify the models, while maintaining accuracy. Advanced simulators such as the PyBaMM and DandeLiion, developed under the Faraday Institution Multiscale Modelling project allow developers to take advantage of the accuracy of physics-based models in a very broad range of scenarios whilst achieving acceptable simulation run-times.

(4) Pack design

Depending on the cell format, hundreds or thousands of cells are arranged in carefully designed and engineered configurations to form a battery pack to deliver voltage and power to the car. The BMS, which monitors the health and performance of these cells, makes extensive use of different analytical pack-level models to ensure safety. Examples include thermo-electrical modelling of 2D and 3D systems to extrapolate battery behaviour, fault diagnosis and thermal management. Models are also used to regulate the battery temperature, by deploying cooling systems to keep temperatures within a set operational window, which improves battery performance, driving range and life.

(5) System design

At a system, national or global scale, techno-economic models, which assess the costs and benefits of using a technology for a particular application, are useful to assess the suitability and impact of a technology as a system-wide deployment and across its lifetime operation. Insights gained from the use of techno-economic models are useful, for example, for informing policy decisions, the optimal interaction of EVs with the grid, optimal charging mechanisms or comparing lifecycle greenhouse gas emissions of two competing technologies.

Compromising between detail and runtime

Computer models need to have reasonable runtimes in the order of minutes or seconds to be useful for researchers and battery designers, but there is often a trade-off between accuracy and runtime. The larger the system, or the longer the length scale being modelled, the more interactions between components need to be tracked, adding to the computational time. If models could keep track of all the interactions between all atoms in a cell over long periods of time, then they would always be able to reliably predict cell behaviour. While this level of accuracy and detail is desirable, the computation time required to run this process for larger scales, such as whole cells, would take too long and involve substantial costs through the intensive use of expensive supercomputing facilities.

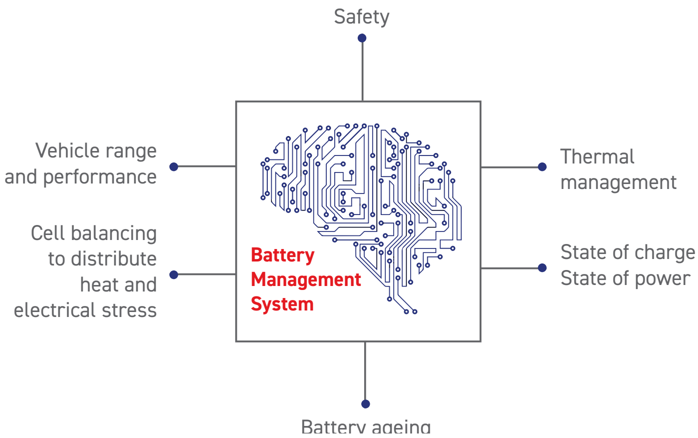
Models to Optimise Battery Performance and Safe Operation

Battery management systems

Battery management systems (BMS) perform a range of important functions to optimise battery performance and ensure safe operation. In particular, the BMS controls battery operation to prevent thermal events that, once triggered, can propagate rapidly. Figure 6 shows the range of functions that a BMS needs to perform. It needs to estimate and keep track of a range of characteristics in order to respond in a way that optimises the behaviour of the battery pack for performance, safety and/or longevity.

Being able to reliably predict battery performance decline or failure often requires knowing the internal variations of, for example, temperature throughout the cell. While sensors can be placed at certain points within the pack to report temperature, it is costly and difficult to insert sensors inside the cells themselves without disrupting their function. Battery simulations are therefore the only way at present to estimate internal conditions and predict behaviour ahead of time.

Figure 6: Functions of a battery management system



Reduced order models for battery pack management

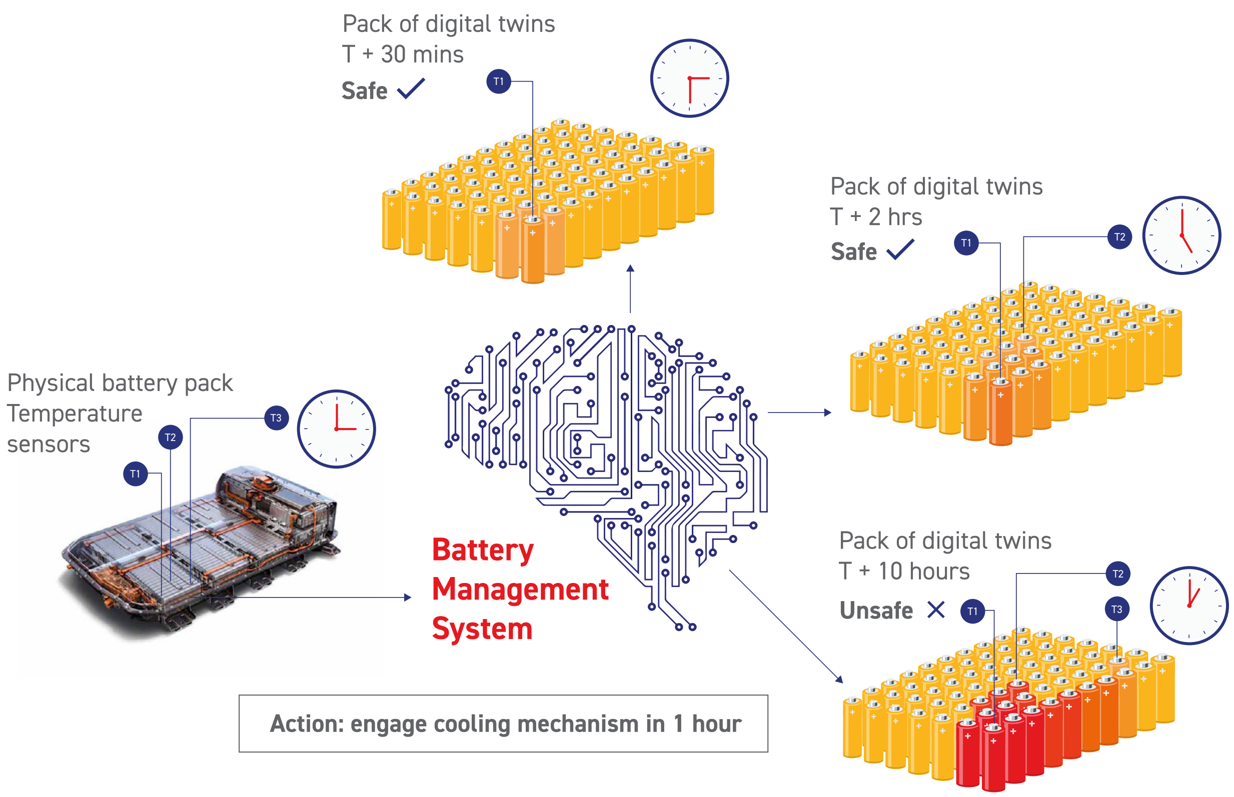
A reduced order model is a simplification of a more detailed model, but with an acceptable loss of accuracy. A digital twin (see Box 4) for each cell in the pack would be a great asset to the BMS, since key features, such as state of charge, power capability and remaining useful life, cannot be directly measured. The digital twin can fill in the gaps by combining the limited measurements made with an accurate prediction of the behaviour. Since a pack is only as strong as its weakest cell, all cells should be represented. However, given that running a digital twin for every cell requires powerful computational capacity, further research into ways to speed up these models is needed.

Box 4: Emerging technology: a battery's "digital twin"

The ultimate aim is to develop a digital twin: a virtual model or set of models designed to accurately reflect the physical battery and predict its performance over time. These virtual models could be run alongside the battery in operation (e.g., in EVs). The digital battery is informed by real world live data from the physical battery to synchronise and validate its models. This enables both the end user and the BMS, see Figure 7, to make decisions about its operation, such as whether fast charging is appropriate, or if the battery life needs to be preserved through a slower charging cycle, or if it is safe to continue to operate the battery in the same way. Digital twins have been successfully used in BMS to improve performance[12] and reduce overall costs.[13]

Billy Wu, at the Dyson School for Design Engineering at Imperial College London, is researching the benefits of creating a battery digital twin. By combining recent advances in battery modelling with an understanding of how batteries degrade over time, the performance and longevity of the physical battery can be optimised while deployed in an EV.[14,15]

Figure 7: Use of a digital twin in a BMS to avoid dangerous or damaging operation



Long-term prediction

The economic attractiveness of the EV battery market will be improved by long-term prediction of battery behaviour, particularly how safe the battery is to run and how long it will last under specific conditions. Accurate digital diagnostics allow researchers to account for some of the uncertainty around battery performance and improve the control systems that operate the battery. Models of battery degradation also help researchers to determine how to extend the usable life of batteries.

EV batteries are evolving so fast that detailed information on battery performance over their lifetime is not yet available in large enough sample sizes and can only be predicted using accurate modelling tools. These models are valuable because they give automotive manufacturers confidence to offer warranties on characteristics such as battery life, performance and total mileage. The case study below shows how Altelium has successfully applied battery models and artificial intelligence (AI) tools to this challenge.

[12] Hyundai news release, Hyundai motor group pilots digital twin technology to improve EV battery performance, May 2022.
[13] General Electric website, This "digital twin" of a car battery could deliver new hybrid vehicle into your garage, May 2016.
[14] B Wu et al, Battery digital twins: Perspectives on the fusion of models, data and artificial intelligence for smart battery management systems, Energy and AI, Volume 1, 2020.
[15] J Reniers et al, Unlocking extra value from grid batteries using advanced models, Journal of Power Sources, Volume 487, 2021.

Box 5: Using models to predict battery failure

Professor David Howey of the University of Oxford has developed a model that accurately predicts solar off-grid battery failure up to three weeks before actual failure. This is based on analysing more than 100 gigabytes of data from more than 1,000 batteries in sub-Saharan Africa.[16] This would enable potentially dangerous batteries to be removed before they cause a safety incident, thereby protecting local communities and allowing equipment manufacturers to optimise their maintenance regimes.[17,18]

Box 6: Altelium: lifetime prediction and risk assessment for the insurance sector

Under the leadership of Professor Harry Hoster, Charley Grimston and John Pesmazoglou, a team at Lancaster University founded Altelium. The company is based on a diagnostic toolkit that simulates chemistry-related battery failure using real-time data and AI tools. This simulation provides the depth of measurable data needed to underpin warranty or investment decisions in EV batteries.

Altelium's platform provides fast and accurate diagnostics to determine the current state of health of the battery and predict expected future performance under different usage conditions. This helps battery users make investment and operational decisions about new batteries, ensuring safe use and maximum lifetime. By linking the electrochemical kinetics of battery degradation with actuarial risk calculations, Altelium's toolkit offers automated pricing and underwriting of insurance products, mitigating financial risk and enabling dynamic new warranties to be offered for first and second life users. Altelium also offers service contracts and operational data to automakers, fleet managers, facility managers and power management companies.[19]

Scaling Up Battery Impacts Through Whole System Models

Adoption of a new technology always brings new challenges. At the scale of an individual installation, a new technology may appear to be the ideal solution, but there are factors that may only become clear when the whole system-wide and global implications are considered. There are many complex interdependencies to factor in when choosing, for example, which type of battery to deploy for a particular application. Whole systems modelling can answer these questions and guide technology choices, whether the aim is to choose the most cost-effective solution or maximise sustainability.

Box 7: The role and value of energy storage in grids

A series of reports[20,21,22] by Professor Goran Strbac at Imperial College London looked at the value of energy storage systems at a whole systems level, modelling the savings that energy storage enables by providing flexibility in how and when energy is used, supporting a larger proportion of renewable generation. The modelling demonstrated that storage generates benefits across the electricity industry, including for generation, transmission and distribution. Benefits are delivered through energy storage applications such as real-time balancing of demand and supply and network congestion management, as well as reducing the need for investment in system reinforcement.

Techno-economic models: system and market-scale impacts

The true cost of any technology is not only dependent on capital and operating expenditure but also on other lifecycle costs such as disposal and clean-up. There may also be cost savings in relation to synergies with other systems and resources, or in comparison with incumbent technologies. The case study below shows how modelling identified energy storage as an important technology to progress for both government and industry.

Market and supply chain risks can be assessed through techno-economic modelling. For example, how the increasing number of EVs interacts with the size and shape of the charging infrastructure required, the implications of EV charging on the energy distribution network or the value of different charging installation strategies. The techno-economic model in this latter case could, for example, examine different charging speeds with respect to the charging time required and the cost of charging stations. These market and policy issues have inspired detailed research and modelling into battery charging behaviour.[23]

Ensuring batteries are sustainable and safe

Batteries are hailed as the enablers of green transport, but modelling is useful to assess the impact of their adoption across the entire lifecycle. While EVs produce few emissions during the use phase, environmental impacts across the full lifecycle from raw material extraction to end-of-life recycling need to be considered.[24] Alternative abundantly available materials together with environmentally benign manufacturing and end-of-life treatment processes are sought to ensure a truly sustainable energy transition. Whole systems models can be used to holistically assess

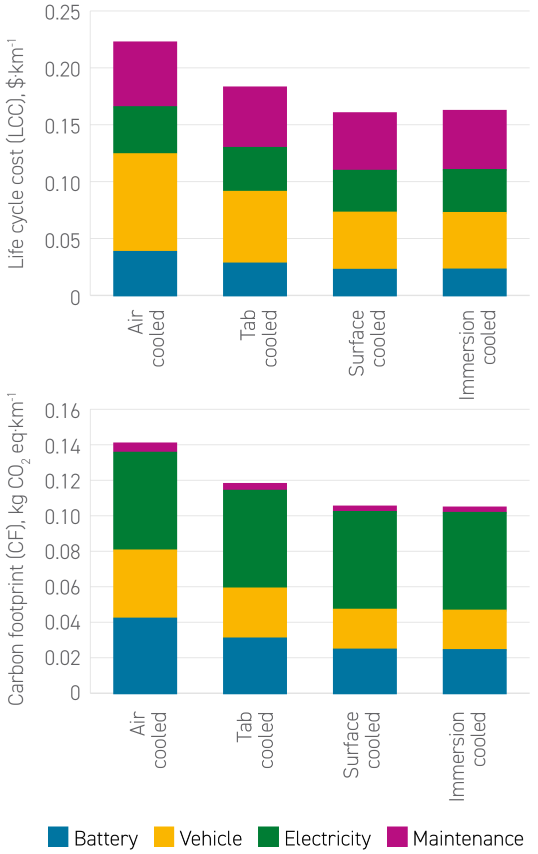
[16] A Aitio and D Howey, Predicting battery end of life from solar off-grid system field data using machine learning, Joule, Volume 5, Issues 12, P3204-3220, December 2021.
[17] Samsung website, Samsung expands recall to all Galaxy Note7 devices, October 2016.
[18] The Independent, Batteries exploding in burning abandoned Illinois building, July 2021.
[19] Faraday Institution success story, Developing diagnostic models to warranty batteries, September 2020.
[20] G Strbac et al, Strategic assessment of the role and value of energy storage systems in the UK low carbon energy future, 2012.
[21] Carbon Trust report, Energy storage report: can storage help reduce the cost of a future UK electricity system? March 2016.
[22] Carbon Trust news release, Groundbreaking analysis reveals a fully flexible energy system could cut the cost of reaching net zero by up to £16.7bn a year in 2050, May 2021.
[23] See for example: Element Energy (March 2019). Electric Vehicle Charging Behaviour Model.
[24] Faraday Insight 9, The importance of coherent regulatory and policy strategies for the recycling of EV batteries, September 2021.

Box 8: Quantifying the benefits of thermal management

Thermal management systems play a significant role in battery engineering as they ensure optimal battery performance and safety. Understanding the impact of cycling on cell and pack temperature regulation and how to slow battery degradation are important research areas. However, it is equally important to understand their whole system impacts, as thermal management systems extend battery lifetime and, in turn, reduce life cycle costs and environmental impacts.

A recent study[25] demonstrates the symbiotic interplay of models at various scales, combining cell-based thermal and degradation models with application scale techno-economic and life cycle assessment models. For example, one model shows that using advanced thermal management systems, such as tab cooling instead of air cooling, reduces the life cycle cost and carbon footprint by 40% and 35%, respectively.

Figure 8: Whole life cycle impacts of different thermal management systems



The analysis differentiates the portions of the lifecycle cost and carbon footprint due to manufacture of the battery and vehicle, the electricity used to charge the battery and any maintenance impacts.[25] Numerical data for figure

relative costs and benefits between different materials and processes.

Considering safety issues is another use of whole systems models. Risks across the battery value chain occur in areas such as the use of toxic chemicals during materials processing, the impact of high battery voltages and from potential thermal runaway reactions leading to fire.[26] Whole systems models will also be useful in guiding recycling strategies and the logistics required for second life use and end-of-life management.

Designing Better Batteries

The challenge for improving batteries is to optimise four key requirements at a system level:

a. Cost (to produce, operate and maintain)

b. Sustainability (recyclable, uses abundant, non-toxic materials)

c. Performance

d. Safety

To improve batteries in one or more of these areas there are multiple avenues that a combined modelling and experimental investigative approach can guide. At the cell level, new materials and chemistries, cell geometries, type and shape of components are just a few examples of variations to explore. Enhancing energy and power performance, for example, could be achieved through different electrode materials or new manufacturing methods, while lower costs could be attained by using more abundant easier to obtain constituents. At the pack level, new pack designs and configurations, combinations of technologies working together, thermal management and charging control algorithms are examples of elements that can impact performance and lifetime. For example, engineering solutions, such as temperature control techniques, could extend lifetime and performance by minimising temperature extremes. At the lifecycle scale, supply chains, manufacturing methods and local energy sources can all be altered to achieve improvements in cost, resource efficiency and sustainability.

Modelling is much more cost effective than experimental methods. Assessing new designs by experiment requires researchers to make a prototype battery cell or pack and run tests on it in a trial-and-error fashion. This wastes expensive materials and is time-consuming. With the fast rate of growth in battery markets, the need for speed in defining optimal battery solutions is especially important. Modelling the complex interdependencies between the factors help researchers explore the possible range of scenarios rapidly and with minimal cost, enabling them to select the most appropriate physical prototype to verify the model results.

[25] L Lander et al, Cost and carbon footprint reduction of electric vehicle lithium-ion batteries through efficient thermal management, Applied Energy, Volume 289, 2021.
[26] Thermal runaway is a particular issue for batteries disposed (unlawfully) in landfills, where degraded cells might overheat and could ultimately ignite landfill fires, which are highly polluting and difficult to extinguish.

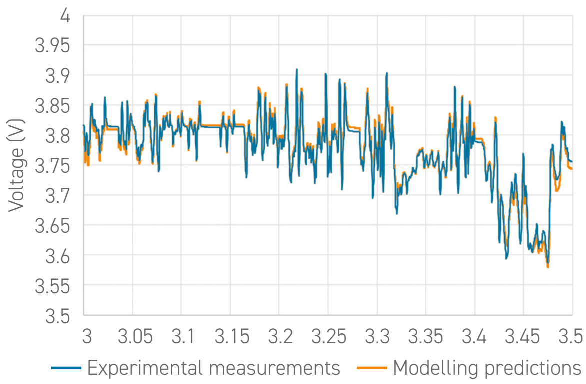
Box 9: The Faraday Institution's Multiscale Modelling Project's design tools

Two modelling platforms, PyBaMM and DandeLiion, have emerged from the Faraday Institution's Multiscale Modelling research project.[27]

PyBaMM[28] is a research tool focused on accelerating the exploration of new ideas. Researchers, including at the University of Oxford, have developed a modular framework for battery models at the cell scale, lowering the barrier for new modellers to explore their ideas in this robust code library. The developers provide accessible support for new users, including online training and documentation.

DandeLiion[29] is commercial software to quickly guide design decisions. Researchers at the Universities of Southampton and Portsmouth have developed a fast, versatile and powerful modelling tool to accelerate battery pack design and deliver improvements to commercial battery performance, lifetime and safety.

Figure 9: DandeLiion rapidly and accurately reproduces experimental results[30]



Box 10: The Faraday Institution's TOPBAT project

TOPBAT, a Faraday Institution funded project in collaboration with AMTE Power, allowed Professor Gregory Offer and his research group at Imperial College London to develop a 3-dimensional, thermally-coupled equivalent circuit model for geometric design optimisation. The model enables thermal considerations to be part of the cell design process, before the first cell prototypes are manufactured. This allows the designer to optimise geometric parameters such as length, width and thickness of a certain cell to be used with a specific thermal management system. Computational efficiency was critical, because cycling through many geometric variations could easily become a very computationally expensive procedure.

Conclusions and Outlook

Battery modelling is increasingly important to battery and EV developers because it facilitates faster and cheaper development of lithium-ion battery packs and improves battery management systems leading to cheaper battery warranties. Decreasing battery development costs is particularly important for SMEs targeting niche markets where extensive and costly development cycles are untenable. However, many companies lack access to high quality, computationally cheap and non-proprietary modelling software with reliable standards.

Developing models to meet these needs is challenging because batteries are highly complex systems requiring different types of modelling at various levels of analysis, including: atomistic models, higher scale models, whole cell models, pack-level digital twins and whole systems techno-economic models. The Faraday Institution's research programmes are making significant progress on developing modelling skills, capability and capacity both for the UK and globally.

With the benefits of physics-based modelling comes the challenge of creating complex models of the cells themselves. To meet this challenge, the Faraday Institution is working with industry to explore an open, standards-based approach to drive seamless interoperability of physics-based battery models; initially for PyBaMM and DandeLiion, but with the intention that the standard should be straightforward to adopt for other physics-based simulators. The aim here is to reduce fragmentation and costs to industry, facilitate agile development and maintain a world-class and evolving standard for the future.

A further challenge to the reliability of battery models is the accuracy of their input parameters, which is a complex issue because battery performance has many interdependencies. A spin out of Imperial College London and the University of Birmingham, About:Energy, has expertise in extracting the experimental data required to construct battery models - an activity known as parameterisation.[31] An increasing number of UK-based companies are exploiting About:Energy's extensive knowledge in this area, which is the first parameterisation company to support the new standardised approach proposed by the Faraday Institution.

Battery modelling opportunities in the UK could be further boosted by:

- **The adoption of standardised approaches** to support the wider use of physics-based models to provide accurate prediction of battery system performance.
- **High speed computing facilities that run battery models.** This will allow the properties of many more materials to be determined and assessed for suitability.

[27] Faraday Institution success story, Ultra-fast software models to accelerate battery design development, March 2021.
[28] PyBaMM website.
[29] DandeLiion website.
[30] A Zülke et al, Parametrisation and Use of a Predictive DFN Model for a High-Energy NCA/Gr-SiOx Battery, Journal of The Electrochemical Society, Volume 168, Number 12, 2021.
[31] Faraday Institution news release, Commercial UK battery modelling capability to speed up battery development in UK, January 2022.

- **Robust data collection from batteries.** This will enhance the understanding of battery behaviour and improve the accuracy of battery modelling, by providing much-needed validation.
- **Support for atomistic research and development.** This modelling is key to understanding why batteries degrade and which conditions accelerate the process.
- **Standardisation of experimental techniques.** This includes the use of standardised testing and data processing procedures across academia and industry, for parameterisation and diagnostics.

Battery modelling is making substantial practical contributions to predicting battery performance and the chance of battery failure. This will help to improve the performance, longevity, safety and sustainability of batteries and enable a smooth transition of the UK to a green economy.

About the Faraday Institution and Faraday Insights

The Faraday Institution is the UK's independent institute for electrochemical energy storage research, skills development, market analysis, and early-stage commercialisation. We bring together academics and industry partners in a way that is fundamentally changing how basic research is carried out at scale to address industry-defined goals.

Our 'Faraday Insights' provide an evidence-based assessment of the market, economics, technology and capabilities for energy storage technologies and the transition to a fully electric UK. The insights are concise briefings that aim to help bridge knowledge gaps across industry, academia and government. If you would like to discuss any issues raised by this "Faraday Insight" or suggest a subject for a future Insight, please contact Stephen Gifford.

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We acknowledge funding from the Policy Support Fund, part of UKRI QR funding, in 2020/21.

https://doi.org/10.25561/101016

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