Institution: University of Portsmouth		
Unit of Assessment: UoA 10: Mathematical Sciences		
Title of case study: Improving lithium-ion batteries for electric vehicles through mathematical modelling		
Period when the underpinning research was undertaken: 2016 to present		
Details of staff conducting the underpinning research from the submitting unit:		
Name(s):	**Role(s) (e.g. job title):**	**Period(s) employed by submitting HEI:**
Dr Jamie Foster	Reader in Applied Maths	01/06/2016 - date
Period when the claimed impact occurred: 2016 to present		
Is this case study continued from a case study submitted in 2014? N		

1. Summary of the impact

Foster has equipped industry with enhanced theoretical understanding and modelling capabilities that, in the words of [text removed for publication] (S1), have provided "significant economic benefit" by decreasing "overall development cost" of manufacturing battery modules for electric vehicles (EVs). The lithium-ion battery (LIB) industry is currently worth USD40 billion per year, predicted to be USD92 billion per year by 2024. The impact has primarily been realised via changing practices at GM who are increasing their investment in LIBs to >USD27 billion and plan to produce and sell >1,000,000 EVs in 2025.

Foster's work contributes to increased rates of adoption of EVs by enhancing commercial viability of the LIB packs which comprise ~40% of the cost of the EV. These batteries are longer-lasting, safer, charge more quickly, and can be driven further between recharges. This is significant in the context of policies to ban the sale of combustion engines across large portions of the world over coming decades (e.g., UK Road to Zero policy). It will make a major contribution towards societal goals to reduce CO_2, NOx and particulate emissions mitigating climate change and reducing the effects of other pollutants on human health.

2. Underpinning research

Since joining Portsmouth in June 2016, Foster has extensively researched LIBs in collaboration with **General Motors Global R&D** (GM) staff and GM-funded researchers at **McMaster University**. Foster also works under the auspices of the **Faraday Institution**, a key part of the UK Government's Industrial Challenge.

EVs are seen as part of the solution for two of the four Grand Challenges in the UK’s Industrial Strategy: *helping reduce carbon emissions and generating clean growth* and *changing the future of mobility*. The switch to EVs is recognised as crucial to meet the UK’s net zero emissions target by 2050. LIBs are a key component of EVs. They are the technology of choice due to their high energy density (up to 265 watt-hours per kg; around 7 times the density of traditional lead-acid batteries) and have high power densities. Customer hesitation in adoption of EVs arises from several issues, chief amongst them being (i) **lifetime**, the warranty period for LIB packs is typically quoted as 100,000 miles or 10 years (ii) **(dis)charge rates,** the relatively long time required to “refuel” EVs is tens of minutes rather than a few minutes for combustion engine vehicles and (iii) **capacity**, the limited range per recharge. The battery comprises ~25% of an EV’s weight and accounts for ~40% of its cost, making it arguably the most important component. Increases in battery energy/power density will reduce their weight, meaning longer range. Reducing battery degradation will extend useful lifetime, directly reducing cost to consumers and reducing environmental harm from disposal and recycling of EVs. Such improvements are achieved through better design, underpinned by powerful modelling and simulation tools, and also have the knock-on effect of reducing environmental harm due to disposal and recycling of EVs. Foster’s expertise and individual research contribution (mathematical modelling) complements that of his collaborators for outputs (R1-6) who are non-mathematicians (chemists, engineers, practitioners) plus a pure mathematician.

<u>Impact strand 1: Lifetime extension (R2, R4, R5, R8)</u>

Batteries are repeatedly cycled (charged and discharged) over their lifetime, and their microscale mechanics plays an important role in their degradation. However due to LIBs’ highly complex morphology, changes can be difficult to quantify meaningfully. Motivated by state-of-the-art Scanning Electron Microscope (SEM) images harvested by the GM funded imaging group at

McMaster (Canadian Centre for Electron Microscopy), Foster's contribution (R8) was to quantify changes that occur within batteries as they are cycled (Fig. 1, left). The team then developed an approach (using systematic homogenization) where microscopy images of real battery electrodes with a complicated structure are distilled down to a set of scalar measures (effective transport properties) that can be tracked over time (R8). It is now possible to precisely quantify the effects of battery use throughout their lifetimes. We can also identify operating protocols and designs that enhance battery health and lifetime. [Text removed for publication].

Foster's subsequent work exploited these tools to develop a modelling framework that can not only assess but also predict in advance which novel device designs and manufacturing processes will yield LIBs better able to withstand structural damage (Fig. 1, right). Since damage reduces performance and lifetime, it is of major concern to GM and the LIB industry at large. Foster, funded by (G1), designed the physics-based models to allow specific recommendations to be made on (a) the shape and material properties of internal components and (b) the manufacturing processes required to mitigate structural fatigue and extend usable lifetimes (R2, R4, R5).

Figure 1: Left, an SEM image of the complex microstructure within an electrode that is distilled into a scalar parameter by Foster's methods (R8). Right, stresses around an electrode particle, predicted in-silico by Foster's model (R2).

Impact strand 2: Improved (dis)charge rates (R1, R3, R4, R7)

The electrolyte (an ionic liquid) provides the transport pathway for Li-ions between the anode and cathode. For (dis)charge to be sustained, the electrolyte must transport ions at the rate required by the current draw. Foster formulated novel models to account for ion-pairing effects and dendrite formation in these ionic liquids, motivated by two important goals: (i) designing electrolytes with improved transport capabilities for use in high-rate cells, and (ii) avoiding lithium dendrite formation which can cause short-circuiting and, in extreme cases, thermal runaway and catastrophic explosion (R1, R3, R7). Foster has developed optimisation strategies that alleviate a bottleneck in LIB production: electrode drying. LIB electrodes are prepared by applying a coating (of a slurry containing the electrode components) onto a metallic film current collector. This is then dried to remove solvent. There is a commercial incentive to maximise throughput using high rate drying. However, this leads to detrimental heterogeneous internal structures. In (R4) a novel model is used to elucidate the physical mechanisms driving the heterogeneity formation, leading to recommendations on smart drying protocols that can speed up drying without damaging electrode performance.

Impact strand 3: Capacity increases (R3, R6)

More recent work has focussed on the atomic structure of the metal-oxides used as the primary active component of the majority of LIB cathodes on the market today. Informed by experimental data provided by co-authors (R6), Foster developed a computational algorithm for predicting the arrangement of atoms within these materials, enabling more focused interrogation of existing material structures than can be conducted through experiment alone. The resulting improvements in theoretical understanding reveal which features of the atomic arrangements correlate directly with enhanced electrochemical performance. These features can then be incorporated into future material designs (R6). An industrially-relevant strategy for increasing battery capacity is to increase electrode thickness. However this makes Li-ion transport pathways longer, as they navigate between electrodes, hampering high rate discharge. Foster modelled the bespoke charging protocols investigated in (R3) that partially overcome this difficulty, showing that a brief current reversal during (dis)charge helps utilise more fully the capacity of such electrodes.

Impact strand 4: Battery simulation tools

Many of the modelling techniques that Foster developed are embedded within an extremely fast linear-scaling code (**DandeLiion**) which solves the most ubiquitous electrochemical battery model (the Newman model). Foster designed and created the first version, and has continued to provide technical supervision throughout its subsequent development. Owing to DandeLiion's speed and power, others can now perform computations on composite batteries and modules that are not possible on other platforms. DandeLiion provides a digital twin of real batteries allowing industry to cheaply and quickly benchmark novel designs, saving significant development time and money. Foster is being supported by the Faraday Institution to form a spin out company to export DandeLiion across academia and industry as a commercial product (www.dandeliion.com).

3. References to the research

R1	Richardson, G., **Foster, J.,** Sethurajan, A., Krachkovskiy, S., Halalay, I., Goward, G., & Protas, B. (2018). The effect of ionic aggregates on the transport of charged species in lithium electrolyte solutions. *Journal of the Electrochemical Society, 165*(9), H561-H567. https://doi.org/10.1149/2.0981809jes
R2	**Foster, J.,** Huang, X., Jiang, M., Chapman, S. J., Protas, B., & Richardson, G. (2017). Causes of binder damage in porous battery electrodes and strategies to prevent it. *Journal of Power Sources, 350,* 140-151. https://doi.org/10.1016/j.jpowsour.2017.03.035
R3	Krachkovskiy, S. A., **Foster, J.**, Bazak, J. D., Balcom, B. J., & Goward, G. R. (2018). Operando mapping of Li concentration profiles and phase transformations in graphite electrodes by MRI and NMR. *Journal of Physical Chemistry C, 122*(38), 21784-21791. https://doi.org/10.1021/acs.jpcc.8b06563
R4	Font, F., Protas, B., Richardson, G., & **Foster, J.** (2018). Binder migration during drying of lithium-ion battery electrodes: modelling and comparison to experiment. *Journal of Power Sources, 393,* 177-185. https://doi.org/10.1016/j.jpowsour.2018.04.097
R5	**Foster, J.,** Chapman, S. J., Richardson, G., & Protas, B. (2017). A mathematical model for mechanically-induced deterioration of the binder in lithium-ion electrodes. *SIAM Journal on Applied Mathematics, 77*(6), 2172-2198. https://doi.org/10.1137/16M1086595
R6	Harris, K. J., **Foster, J.,** Tessaro, M. Z., Jiang, M., Yang, X., Wu, Y., Protas, B., & Goward, G. R. (2017). Structure solution of metal-oxide Li battery cathodes from simulated annealing and lithium NMR spectroscopy. *Chemistry of Materials, 29*(13), 5550-5557. https://doi.org/10.1021/acs.chemmater.7b00836
R7	Sethurajan, A. K., **Foster, J.**, Richardson, G. Krachkovskiy, S. A., Bazak, J. D., Goward, G. R., & Protas, B. (2019). Incorporating dendrite growth into continuum models of electrolytes: insights from NMR measurements and inverse modelling. *Journal of the Electrochemical Society*, *166*(8), A1591-A1602. https://doi.org/10.1149/2.0921908jes
R8	Liu, H., **Foster, J.**, Gully, A., Krachkovskiy, S. A., Jiang, M. Wu, Y., Yang, X., Protas, B. Goward, G. R., & Button, G. A. (2016). Three-dimensional investigation of cycling-induced microstructural changes in lithium-ion battery cathodes using focused ion beam/scanning electron microscopy. *Journal of Power Sources, 306*, 300–308. https://doi.org/10.1016/j.jpowsour.2015.11.108

All outputs are in high-quality internationally peer-reviewed journals, whilst R5 best demonstrates the quality of the underpinning mathematics. The following grants supported the work:

G1	**Foster, J.** (PI) *Multiscale modelling of mechanical deterioration in lithium-ion batteries*. Funded by the Engineering and Physical Sciences Research Council, New Investigator Award. March 2020 - March 2023. (GBP 310,610)
G2	**Foster, J.** (PI) Faraday Challenge *Multi-Scale Modelling Project*. Funded by The Faraday Institution. March 2019 - February 2021. (GBP 231,891)
G3	Goward, G. (PI) (**Foster, J.** named collaborator on proposal) *Structural evolution of electrode materials and mitigation of degradation by Mn-trapping in Li-Ion Batteries via complementary characterization methods and mathematical modeling*. Funded by the Natural Sciences and Engineering Research Council of Canada, 2016-2020, (CAD1,420,000).

4. Details of the impact

The developments above were achieved since Foster joined UoP in June 2016 and have led to improved processes and products within GM, innovation with the Faraday Institution and at McMaster University, and a state-of-the-art software tool now used by practitioners internationally.

From research to impact

General Motors manufactures batteries, employs 164,000 people and serves 6 continents. GM is the first company to mass-produce an affordable EV, the Chevrolet Bolt. Its EVs have been driven 4,200,000,000km, saving 159,000,000l of gasoline and avoiding 312,000t of CO_2 emissions per year. GM's commitment to the EV market is evidenced by their joint investment (with LG Chem) of USD2.3 billion in the EV plant in Lordstown, Ohio, and planned production of 20 new EV models by 2023. The health of the relationship between Foster and GM is evidenced by five joint publications (including R1, R2, R6, R8) with GM scientists and a further two (including R3, R4) directly funded by GM in leading energy journals.

McMaster University has a long-standing relationship with GM. For 8 years GM has funded research at McMaster (with the Natural Sciences and Engineering Research Council of Canada) with an investment of ~CAD8,000,000. Foster is a named collaborator on the most recent renewal of this grant (G3). He supervises GM-funded Postdoctoral Researchers (Drs William Ko, Jose Escalante, Francesc Font and Lindsey Daniels), via his adjunct position at McMaster.

The Faraday Institution (FI) is the UK's independent body for electrochemical energy storage research, skills development, market analysis, and early-stage commercialisation, and acts as a conduit between academia and industry. Foster secured over GBP230,000 from FI (G2) since 2019 and is supported by them to set up a spin-out company around the DandeLiion software.

Nature and extent of impact strand 1: Lifetime extension

Beneficiaries of longer-lifetime and more reliable EVs include industry, motorists and the environment through reduced disposal/recycling. Foster's experimentally-validated model of mechanical changes (R5) equipped GM with the means to test novel designs in-silico without costly and time-consuming prototyping: [text removed for publication] this work "sheds light on the microstructural changes of the battery electrode during cycling. These changes are strongly linked to battery degradation mechanisms and this work has […] opened new avenues for ameliorating these changes, and thereby helped us extend cell life-time" (S1). Altering the drying step provided further lifetime extension techniques (and monetary savings) [text removed for publication]. It is crucial to estimate a device's state-of-health so that it is removed from service when needed. Improperly judging this can lead to internal short-circuits and, potentially, catastrophic explosion. "Our work with Foster… has been crucial in helping us understand, and accurately model, several key aspects of Li-ion battery operation and has significantly increased the impact of our work." (S2). Foster's framework provided better state-of-health estimates enabling timely replacement/repair to prevent unexpected failures (R8). The framework led to a model that supported the GM scientific team "to understand the electrode conductivity evolution during battery cycling. This is an indicator of battery health and this work has helped us understand how to assess health in situ" (S1).

Nature and extent of impact strand 2: Improved (dis)charge rates

Faster charging batteries remove a major deterrent for potential EV consumers who want a 'greener' mode of transport, with knock-on benefits to the environment (through CO_2 emission reduction), and human health in urban areas (by reducing other pollutants). [Text removed for publication].

Nature and extent of impact strand 3: Capacity increases

Higher capacity batteries last longer between recharges, benefitting consumers, transport operators, as well as the industry. Foster "developed… the tool that is required to synthesise higher capacity materials, which will further improve the energy density of Li-ion batteries. For automotive applications the increase of the energy density is of the utmost importance" (S2). [Text removed for publication]. Increasing electrode thickness is a key strategy for GM to manufacture enhanced capacity anodes for EVs. [Text removed for publication]. Thus Foster's research has led to batteries that are not only more efficient, better maintained and longer lasting, but also safer for the consumer.

Nature and extent of impact strand 4: Battery simulation tools

A major fruit of Foster's work is the ultra-fast LIB simulation tool, DandeLiion, which is now used by academia and industry internationally. The Faraday Institution is supporting commercialisation via a spin-out company. Having originally been identified by Faraday Institution due to a need for his coding expertise, Foster's subsequent research presentation to a panel of UK captains of industry was met with enthusiasm for the formation of a spin-out. [Text removed for publication]. DandeLiion's impact to date can be quantified and evidenced by >300 jobs already executed by academic and industrial users internationally (Fig. 2) on its dedicated server (dandeliion.com, S4). [Text removed for publication].

Figure 2 (Right): Geographic reach of DandeLiion: Blue shows active users [Google analytics].

Summary

Foster's research at UoP has armed industry worldwide with enhanced theory, modelling capability and state-of-the art software, that drives down development costs and "has numerous knock-on effects, including by decreasing the waste stream and the burden of recycling" (S1). The work benefits consumers because improved EV batteries are cheaper, safer, longer-lasting, charge more quickly, and can be driven further between recharges. Economic benefits have been delivered to a huge industry (already worth USD40 billion per year and set to experience significant growth). This industry's growth rate and success are crucial in achieving CO_2 emission reductions in the UK and internationally.

5. Sources to corroborate the impact

S1	Factual Statement from [text removed for publication] at General Motors Global R&D. 26/08/2020
S2	Factual Statement from [text removed for publication], McMaster University, Canada. 04/09/2020
S3	Factual Statement from [text removed for publication] at the Faraday Institution. 11/12/2020
S4	DandeLiion: http://dandeliion.com, "Ultra-Fast Online Solution to the Newman Model of Li-Ion Battery Performance", simulation queue: https://simulation.dandeliion.com/queue/