MATHS FOR BETTER BATTERIES

Simple models for battery degradation

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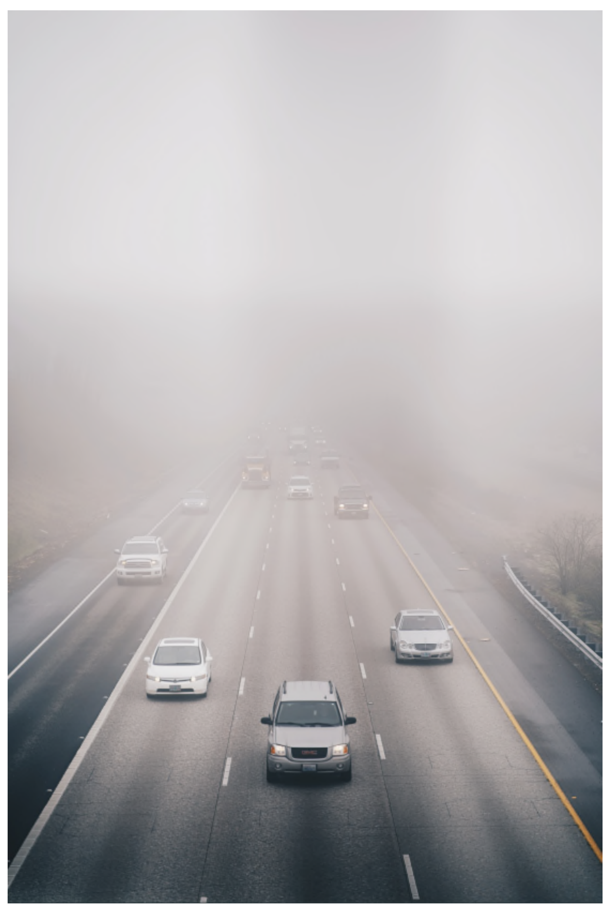
I. AN ELECTRIC REVOLUTION

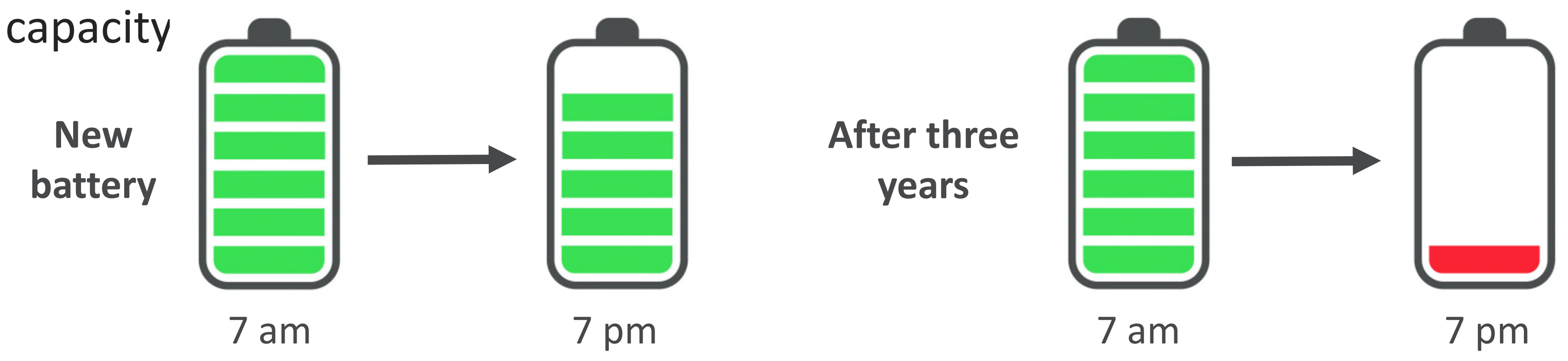
Climate emergency is one of the biggest challenges we face as a society and global policies are needed to revert the situation. In the United Kingdom, the government has committed to reach **net zero greenhouse gas emissions by 2050**. Of all the measures put into place to achieve this goal, probably the one with the biggest impact on our day-to-day lives is the **ban on combustion vehicles from 2030**. The only way for this transition to be successful is through **more durable and efficient batteries**, and mathematical models will play a key role in developing them.



Challenge: Derive fast and accurate models to design durable and efficient batteries that enable the transition to net zero emissions.

II. LIKE HUMANS, BATTERIES ALSO AGE

Battery degradation (or ageing) is a phenomenon that we have all experienced: the battery of a new phone can last days between charges but, after a few years of use, the same battery can only last a few hours. This **decrease in capacity** is caused by battery degradation. Degradation is well documented, but its potential causes are many and **poorly understood**. One of the most reported effects are **side reactions**, in which lithium is consumed to create some new material that blocks the pores in the battery electrodes. This combined effect causes a significant decrease in battery capacity



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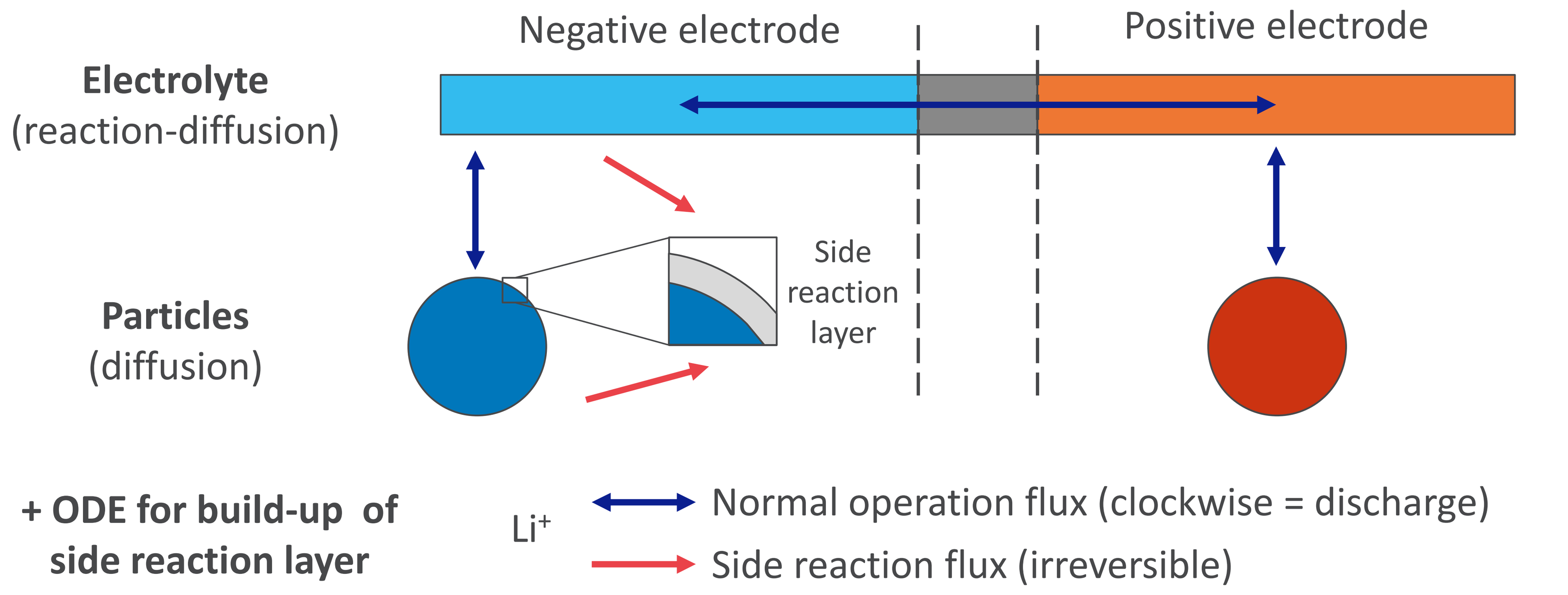
Degradation causes a decrease in the battery capacity, but its **potential causes are many and poorly understood**.

III. A SIMPLE MODEL FOR DEGRADATION

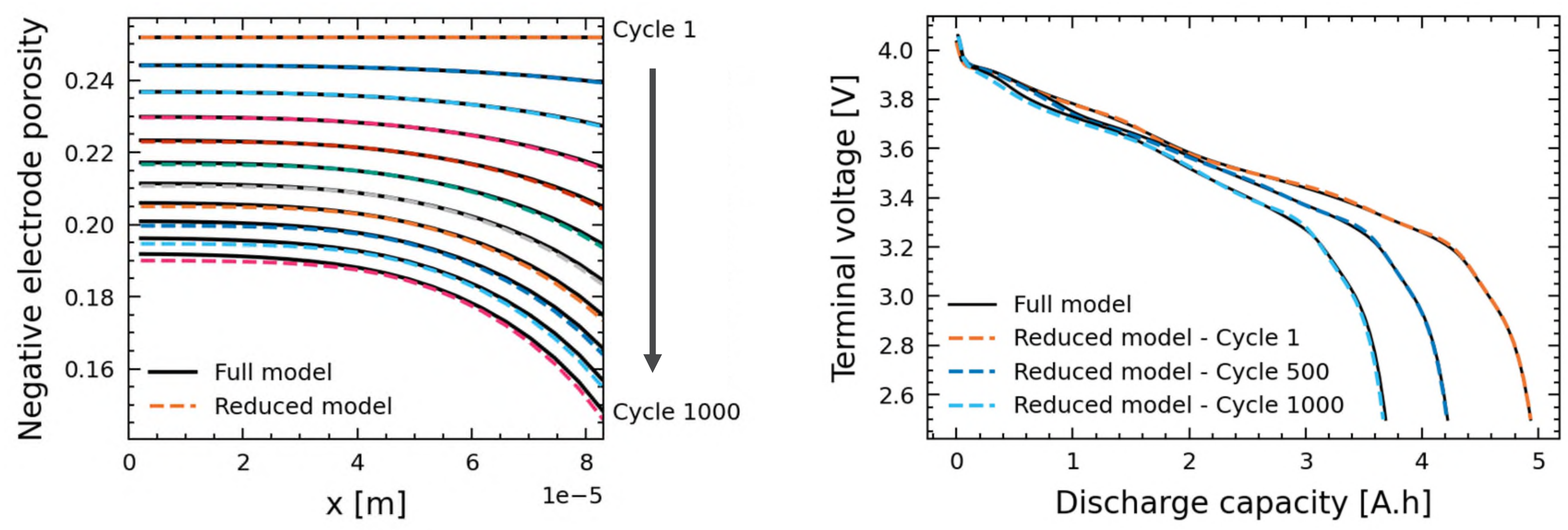
- Degradation models are commonly based on the Doyle-Fuller-Newman model (DFN), which accounts for mass and charge transfer in both the porous electrodes and the electrolyte. These **standard models are too complex for many applications**, so reduced models are needed.
- Reduced models can provide **better theoretical understanding and faster predictions**, without compromising the accuracy.
- We start with a DFN model coupled with a side reaction and porosity change (full model) and perform an **asymptotic analysis** in the limits of weak side reaction and small overpotentials to derive our reduced model.
- The reduced model is **much simpler** than the DFN model, but generic enough to account for a **wide range of side reactions**, including solid–electrolyte interphase (SEI) growth, lithium plating and a combination thereof.



Degradation models are often too complex, so reduced models are needed for **better theoretical understanding and faster simulations**.

IV. 1000 BATTERY CYCLES IN LESS THAN 10 MINUTES

- Both the full and reduced model have been implemented in **PyBaMM, an open-source package for battery modelling**. The models have been tested for different side reactions (SEI growth, lithium plating, and both combined) and different cycling conditions.



Brosa Planella & Widanage (2022), *in preparation*

- The reduced model shows **similar accuracy** to the full model (**< 1% error**) while being much simpler. For identical mesh sizes, the reduced model is **8x smaller** and can run **up to 8x faster**. Because our model is simpler, it is suitable for applications where computational power is limited, such as battery management systems.
- 1000 charge-discharge cycles (4 months of continuous operation time) can be simulated in 8 minutes. This is **20,000 times faster than real time**.
- The reduced model can accurately predict not only **global states** such as capacity and voltage, but also **internal states** such as the porosity distribution.

Our reduced model implemented in PyBaMM (open-source) **shows similar accuracy and is up to 8x faster** compared to standard models.

V. IMPACT TO SOCIETY

We derived a reduced model which can be applied to many demanding applications such as:

- **Design:** choose from a wide range of prototypes before experimental testing.
- **Management:** control the battery operation to improve performance and extend lifetime.
- **Diagnosis:** at the end of life, determine if a battery can be repurposed or should be recycled.
- **Fast charging:** reduce the charging time without damaging the battery.

Fast and accurate models for battery degradation, like the one presented here, are a fundamental tool to develop a new generation of **better and greener batteries** which are called to have a fundamental role in the transition to net zero greenhouse emissions.

Conclusion: Our model provides fast and accurate simulations for battery degradation, which are a fundamental tool to develop better and greener batteries.

RESEARCHER BIO

Ferran is a Senior Research Fellow at the University of Warwick and The Faraday Institution, working on the "Multi-Scale Modelling" project. His research interests are on mathematical modelling with applications to industry, with a particular focus on sustainable technologies. He is also interested in working closely with experimentalists to bring together the outputs of the models and experiments, and help bridging the gap between both disciplines.

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