Modelling Plenary Keynote Abstract & Speaker Biography

Improving performance of Li-S cells in real conditions, a model-informed approach

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A lack of understanding of the complex electrochemical, transport, and phase-change phenomena in Li-S cells is arguably holding back improvements in their performance[1]. At the same time, their successful commercialisation is also dependent on the availability of tools for estimating the state of charge and state of health in the particular application.

For the past three years we have been working as part of the wider Revolutionary Electric Vehicle Battery (REVB) project on using modelling to tackle these challenges. We have developed a variety of models at various scales in order to both help understand the performance of Li-S cells and help monitor and control them. This presentation will guide you through the journey of discovery that we have enjoyed.

Despite the fact that the exact chemical pathways for discharge and charge in a Li-S cell have still to be elucidated [1], much of their behaviour under realistic conditions was shown to be governed by precipitation and dissolution [2]. It is mainly due to the timescales of precipitation that equivalent circuit models in the form used for Li-ion batteries are ill-suited for Li-S estimation and control, as on-going precipitation during discharge affects the measurement of the OCV curves.

Modelling has also enabled us to study the role of electrolyte and species transport on battery performance. We were able to show via a zero dimensional model that in order to retrieve the correct series resistance values, the diffusivity of species must be concentration dependent [3]. This feature is to be expected given the relatively high electrolyte concentrations reached during discharge, but is not currently accounted for in other Li-S models. Using a one dimensional model with the assumption of a viscous electrolyte, we showed that at higher discharge currents concentration gradients can build in the separator. As a result, capacity is temporarily lost by fast discharge and can be recovered by resting the cell. This assumption was verified experimentally [4].

A zero dimensional model accounting for degradation due to shuttle was used to interpret the complex behaviour observed in cycling experiments and to distinguish between reversible and irreversible degradation. This model provides a tool for knowledge based choices between improving performance and sacrificing power or energy, such as through the introduction of recovery cycles. It also allows us to recommend tailored cycling procedures optimized towards specific goals, such as charging for improved cycling efficiency. Finally, it can be used to extract information from non-invasive measurements of cell degradation.

References

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Speaker Biography:

Dr Monica Marinescu graduated in 2012 with a PhD in Physical Chemistry from Imperial College London. Her research focussed on the theoretical description of electrolyte-electrolyte and electrolyte-electrode interfaces for applications such as electrowetting, variable liquid lenses and mirrors.

Since then she has been working at Imperial College on modelling batteries, with a particular interest in how the physical and chemical processes impact battery behaviour in applications. For the past three years she has been working as part of the REVB project developing electrochemical models to help explain the behaviour of Li-S cells under realistic operating conditions and improve their performance.