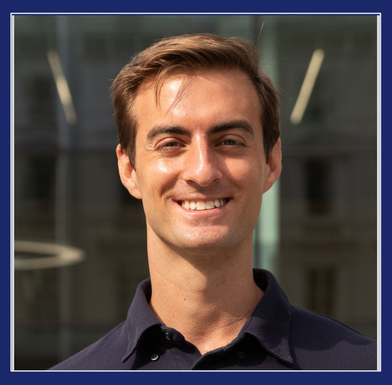
ACHIEVING QUANTITATIVELY ACCURATE LI-S MODELS THROUGH RIGOROUS VALIDATION

A novel predictive zero-dimensional model and testing procedure



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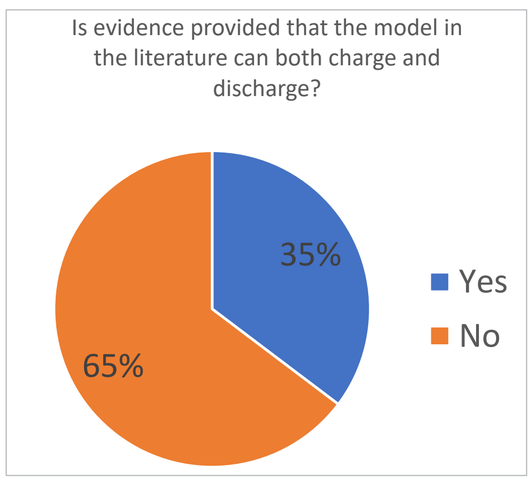
ABSTRACT

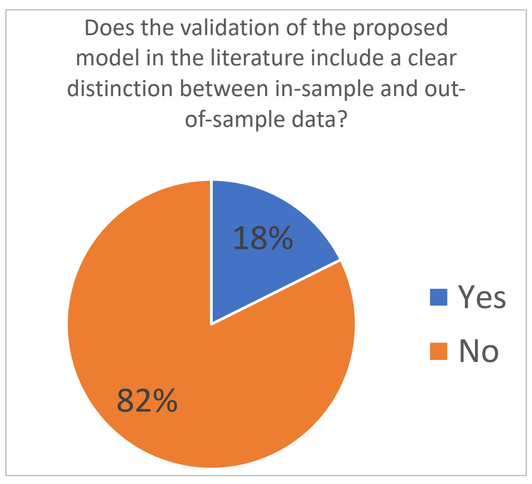
A novel 0D physics-based cell-level model for Lithium-Sulfur batteries is proposed. The model simplifies many of the currently proposed Li-S models while providing strong quantitative performance. Details given in *Cornish & Marinescu* outline and exemplify a proposed empirical model validation procedure which is applicable to both physics-based as well as data-drive models.

- The 0D model provides out-of-sample quantitative predictions for electrolyte resistance.
- *Cornish & Marinescu propose a* Minimum Test Set and Empirical Validation procedure for Li-S cell-level models. The 0D model is validated against this test set.
- The 0D model as well as several proposed models from the literature will be made available as an open-source repository. The models are written using the Python-base PyBaMM library.
- The 0D model is computational inexpensive and can therefore be used in BMS systems.

MOTIVATION

- Achieving quantitively accurate models for Li-Sulfur batteries is still illusive. For example, many papers lack evidence that the proposed models can charge and discharge.



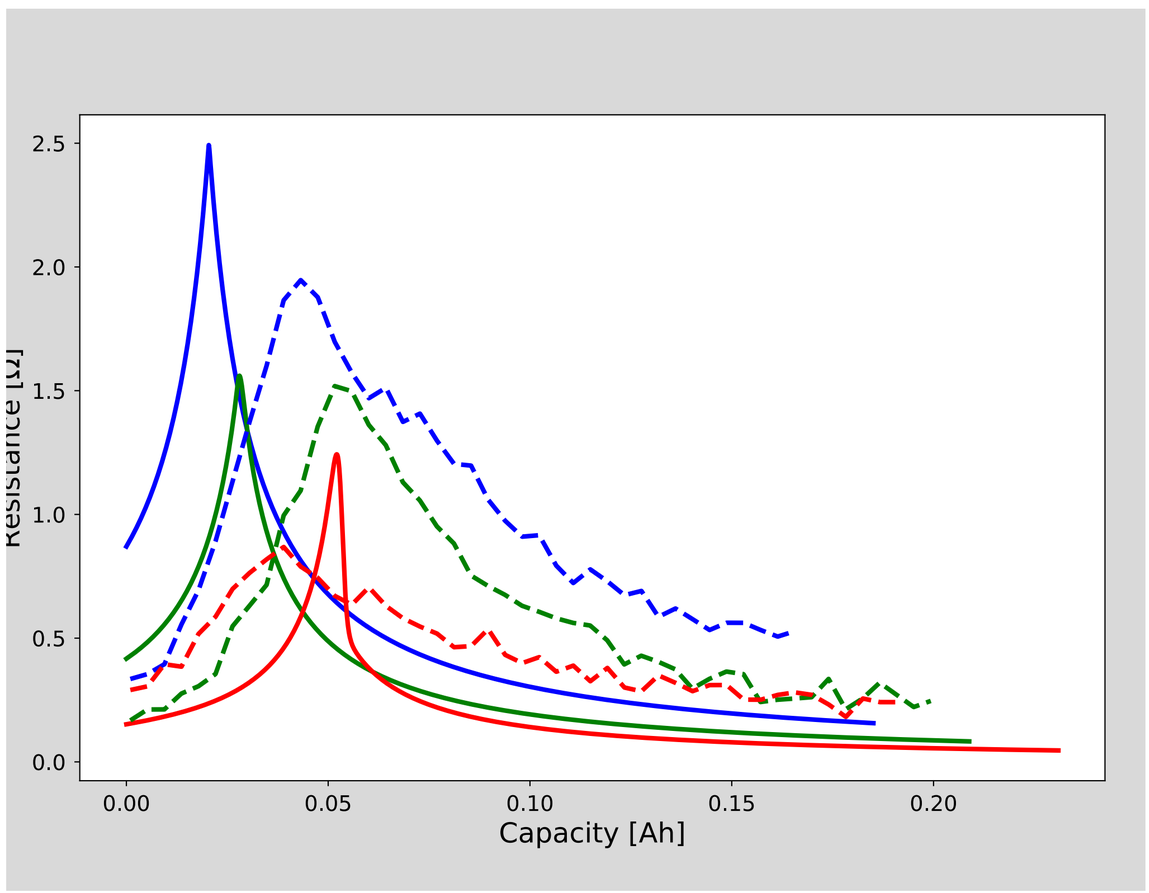


METHODS

- An empirical methodology is proposed to ensure model predictive power is clearly demonstrated for new models. The literature is absent of such rigorous testing procedures.

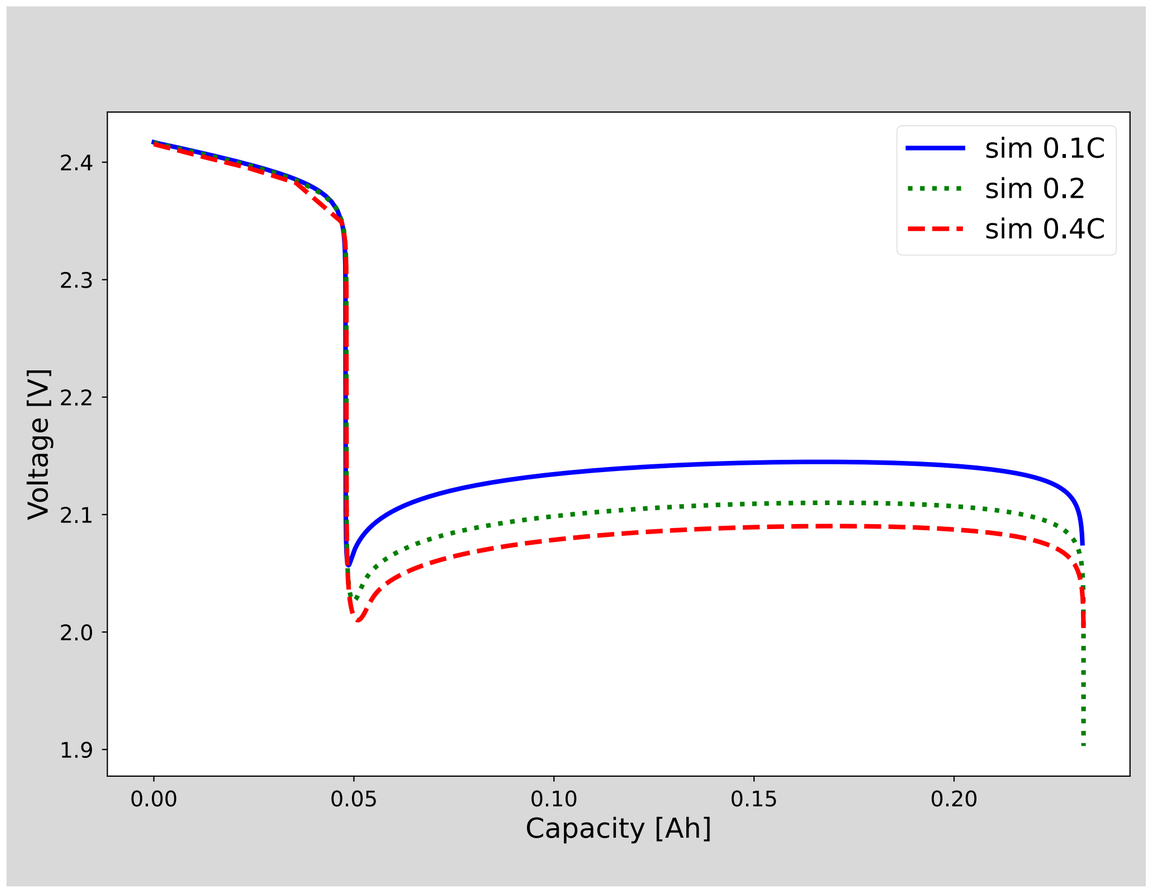
MODEL PERFORMANCE

- As outlined in section 14 of *Robinson et al*., the model validation procedure splits the experimental data into in-sample data, used for model fitting, and out-of-sample data, used for predictive power analysis. Such data splits are necessary to provide evidence that the model can provide information on cell behavior beyond the experimental data set.
- The novel zero-dimensional model proposed in *Cornish & Marinescu* provides quantitatively accurate out-of-sample electrolyte resistance predictions for experimental cells of *Hunt et al*.



CONCLUSIONS

- The testing procedure outlined in section 14 of *Robinson et al*. and exemplified in *Cornish & Marinescu* provides strong evidence for the predictive power of the model.
- Out-of-sample simulations compared against common Li-S cell behaviors indicate the model captures many Li-S phenomena, such as increased over-potential during discharge given lower C-rates.
- Adoption of the model validation procedure will provide clear information towards model accuracy and allow for more direct model comparisons.



IMPACT / NEXT STEPS

- In subsequent work, the model will be improved to indicate which additional necessary features are required to capture further cell behavior.
- The open-source code will allow researchers to quickly modify the model presented here, thereby ensuring rapid model development.
- Along with the adoption of the model validation procedure, an open-access experimental data set will be created in conjunction with the Faraday Institute. This data set will provide a common fitting and test set to ensure models are meaningfully comparable.

REFERENCES

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RESEARCHER BIO

Michael Cornish is a PDRA at Imperial College London and in conjunction with the Faraday Institute.

Michael is interested in rigorous model validation for both Battery Management Systems as well as models which inform the development cycle. With a background in Applied Mathematics, Michael also is interested in model analysis and reduced order modelling.

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