German Aerospace Center
Deutsches Zentrum für Luft- und Raumfahrt, DLR

Institute of Engineering Thermodynamics
Department of Electrochemical Energy Technology

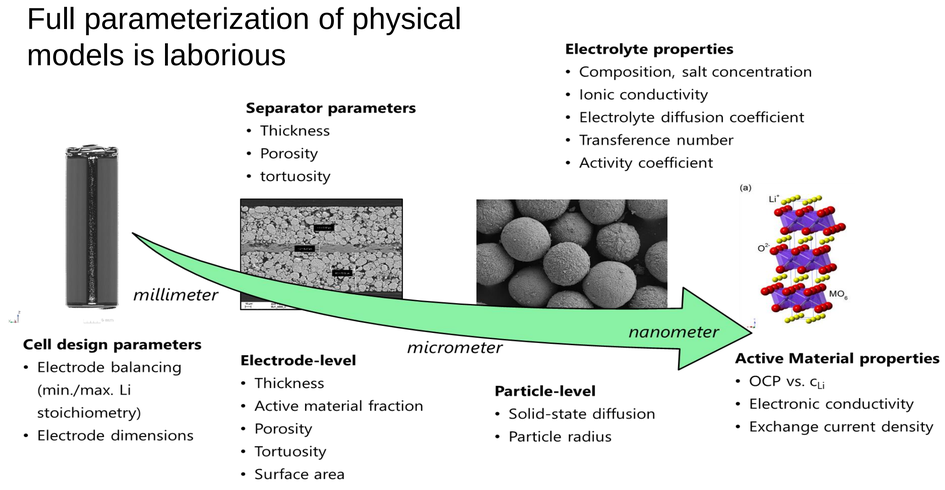
Collaborative Experimental-Computational Workflows For Accelerated Parameterization Of Battery Models

John Mugisa[1], Yannick Kuhn[2], Micha Philipp[2], Eibar Flores[3], Simon Clark[3], Birger Horstmann[2], Christina Schmitt[1], Ruphay Burgos-Frintrup[1] & Dennis Kopljar[1]

1. Deutsches Zentrum für Luft- und Raumfahrt (DLR), Pfaffenwaldring 38-40, 70569 Stuttgart, Germany
2. Deutsches Zentrum für Luft- und Raumfahrt (DLR), Wilhelm-Runge-Straße 10, 89081 Ulm, Germany
3. SINTEF Industry, Battery Technology, Trondheim, 7034 Norway

MOTIVATION

Full parameterization of physical models is laborious



Challenges in model parameterization

- Traditional parameterization is time-consuming and costly
  - Extensive experimental effort,
  - Destructive techniques, specialized equipment and expert knowledge
- Difficulty in extracting reliable parameters from measurements
  - Large variance in literature for same chemistry, thoughtless use of model assumptions

Goal for further development

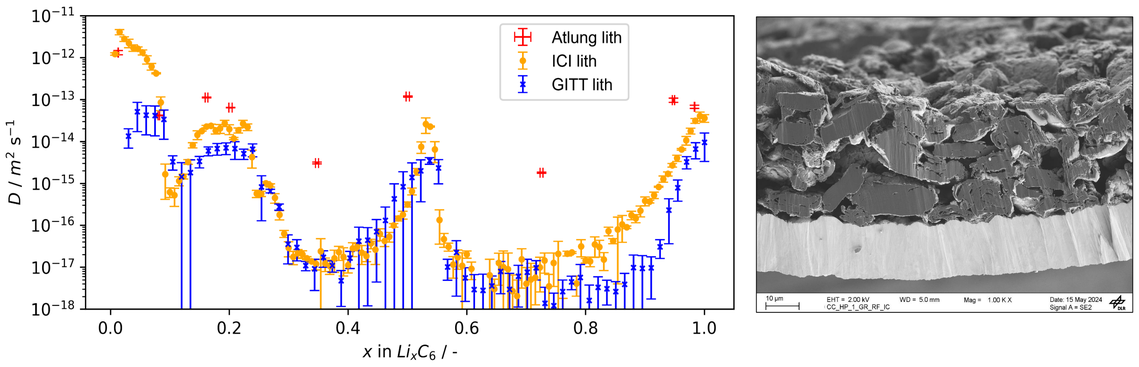
- Need for efficient, automated non-invasive parameterization workflows
  - Reduces time and cost
  - Ensures accuracy and reproducibility

➢ Less parameterization burden can democratize the use of physical battery models

EXPERIMENTS

Experimental sequence for parameter extraction

here: high power commercial graphite electrode



Different state-of-the-art experimental techniques for extraction of Ds have been tested. Results relatively consistent but with huge differences in terms of efficiency: e.g. 120 h (GITT) vs. 20 min (ICI)

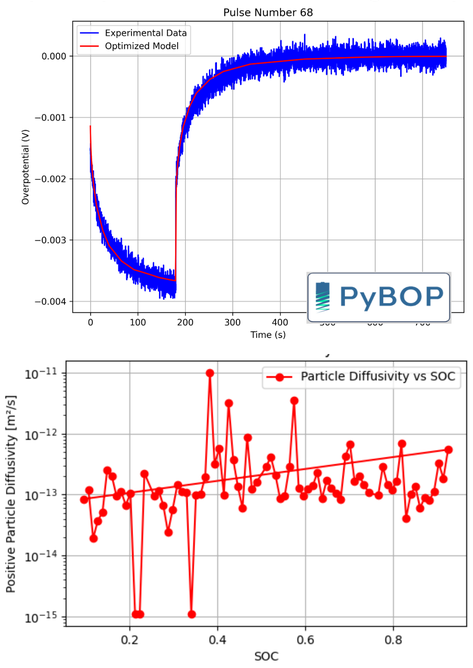
➢ Inherent constraints of analysis models (e.g. Weppner & Huggins) limits the precise capture of underlying mechanisms and meaningfulness of results

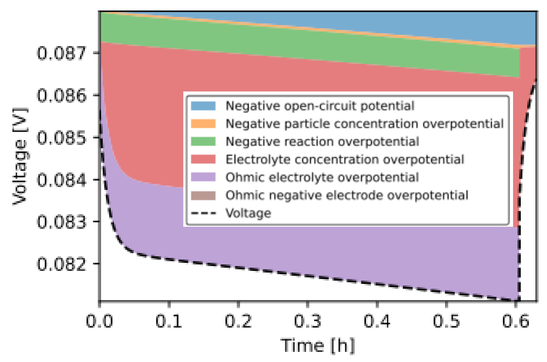
➢ Inverse modeling allows systematic optimization of the experimental sequence and parameters to achieve high accuracy in parameter estimation

INVERSE MODELLING

Model-based analysis to extract parameters

Inverse modelling tools with different functionalities are used: **PyBOP** (Oxford) fits data to all PyBaMM models, while **EP-BOLFI** (DLR) uses Bayesian principles for feature fitting and parameter uncertainty estimation



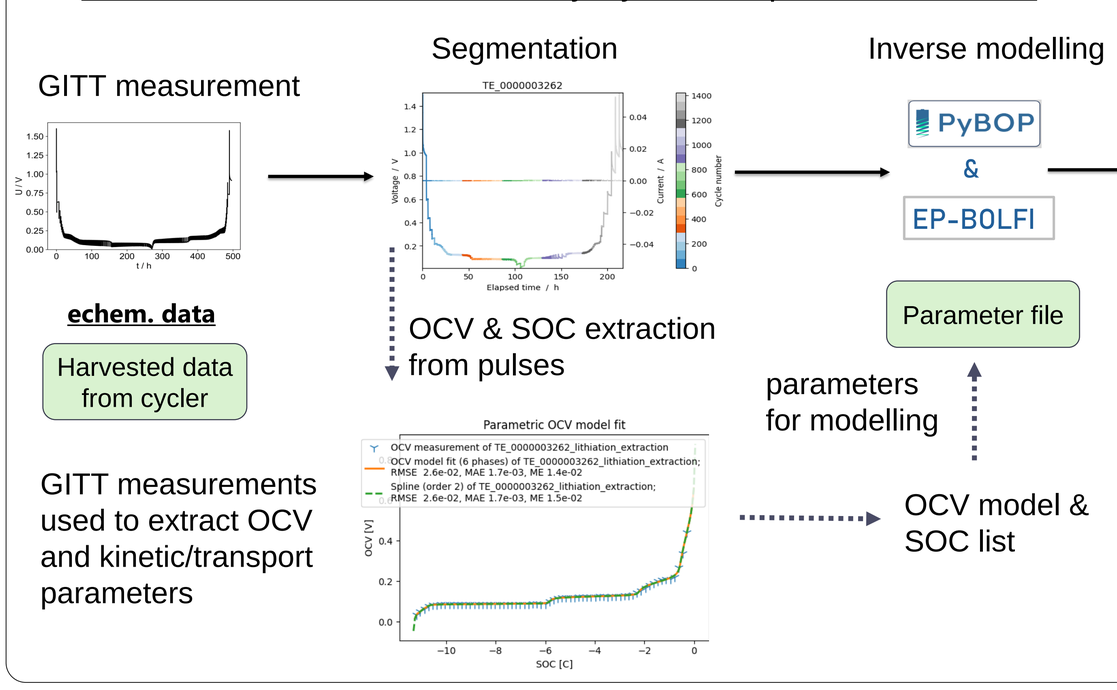


Uncertainty quantification of EP-BOLFI and breakdown of the overpotential contributions shows

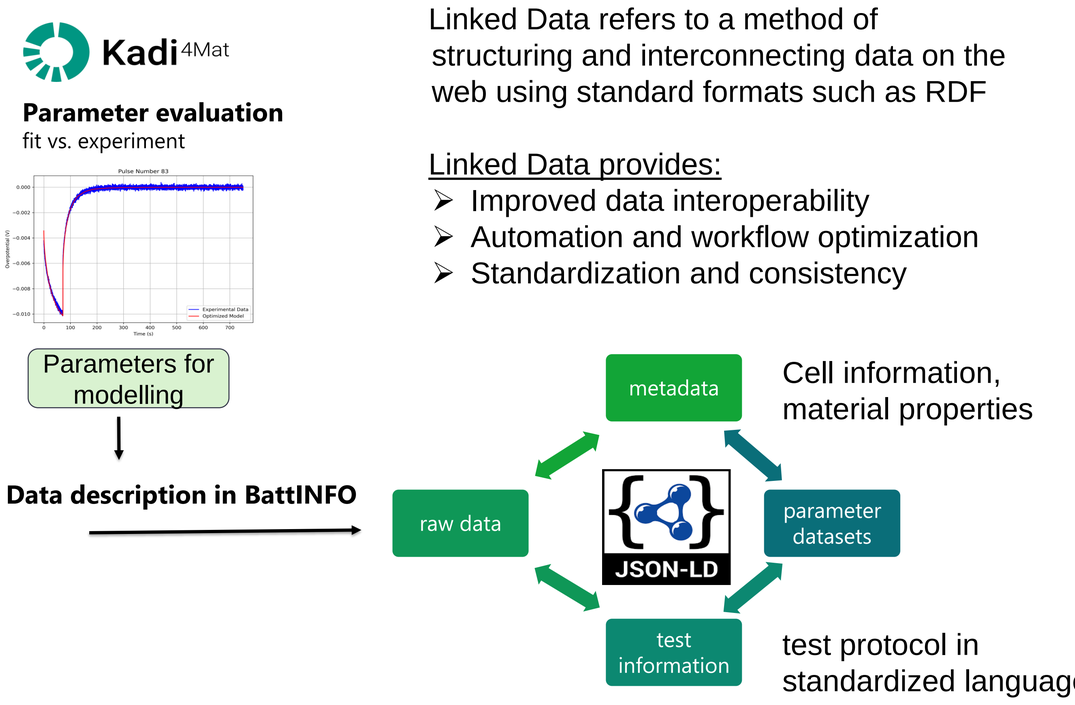
➢ improvement of experimental conditions necessary to obtain more accurate parameters

AUTOMATION

Automated workflows enabled by Python scripts and Kadi4Mat



BATTINFO LINKED DATA



Linked Data refers to a method of structuring and interconnecting data on the web using standard formats such as RDF

Linked Data provides:

➢ Improved data interoperability
➢ Automation and workflow optimization
➢ Standardization and consistency

CONCLUSION

- PyBOP and EP-BOLFI provide robust inverse modeling frameworks with Kadi4Mat ensuring structured data storage and supporting instantiation of workflows
- Standardized data handling in Battery Interface Ontology (BattINFO) ensures accuracy and reproducibility
  - ➢ Utilizes for structured, machine-readable data.
  - ➢ Improves consistency in parameter extraction and interpretation.
- Inverse modelling tools
  - ➢ Systematic study on identifiability and sensitivity of parameters
  - ➢ Optimization of experimental sequence

Acknowledgements

This work is financially supported by the European Commission through the **DigiBatt** project (Funding ID No. 101103997), and we gratefully acknowledge their support. The authors sincerely thank the **University of Oxford** (Prof D. Howey and colleagues) for publicly providing PyBOP and for their valuable support in its implementation.

Deutsches Zentrum für Luft- und Raumfahrt
German Aerospace Center

REFERENCES:

1. S. Clark, F. L. Bleken, S. Stier, E. Flores, C. W. Andersen, M. Marcinek, A. Szczesna-Chrzan, M. Gaberscek, M. R. Palacin, M. Uhrin, J. Friis, Adv. Energy Mater. (2022), 12, 2102702
2. B. Planden, N. E. Courtier, M. Robinson, A. Khetarpal, F. B. Planella, D. A. Howey, PyBOP: A Python package for battery model optimisation and parameterisation, arXiv:2412.15859
3. Y. Kuhn, H. Wolf, A. Latz, B. Horstmann, Batteries & Supercaps (2023) 6, e202200374