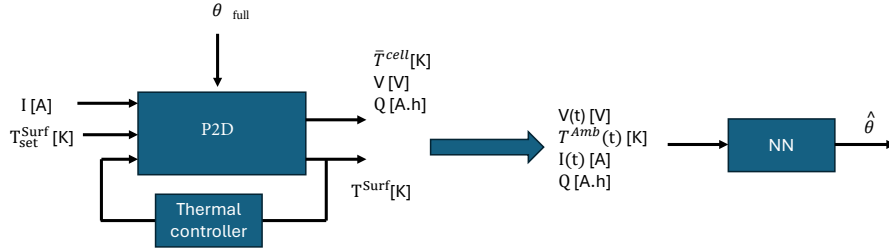


26th Nordic Process Control Workshop (NPCW26): One-shot DFN parameter estimation from timeseries

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Principle overview of data generation and estimation of plant parameters.

Today battery management systems (BMS) commonly describe voltage behavior using state-of-charge-dependent Thevenin equivalent circuits consisting of resistive and capacitive elements [1]. These circuits provide a computationally efficient model with the drawback of not capturing internal electrochemical phenomena. One such phenomenon is a parasitic reaction called lithium plating that occurs at the negative electrode. This process reduces the ionic transport efficiency and causes capacity loss if connection to the electrode is lost [2].

To better describe internal battery behaviour, electrochemical models can be used. A commonly studied model is the Doyle-Fuller-Newman (DFN) model. The DFN model involves a large number of parameters, θ_{full} , that can initially be characterized using equipment available during manufacturing. However, these parameters are time-varying due to aging mechanisms, rendering the initial parameterization invalid.

In this work, a DFN model together with aging models is used to simulate the lifetime of a set of battery cells using Python Battery Mathematical Modelling (PyBaMM) [3, 4]. By varying initial parameters of θ_{full} , different aging trajectories are generated. A neural network (NN) is then trained to estimate a subset of time-varying parameters, $\theta \subset \theta_{full}$. Simulated aging trajectories of θ are used as validation, while additional training data is generated by preserving rank correlation of the target trajectories and simulating individual charge cycles. NN input features are selected such that they should be available during practical operation for an existing BMS. By estimating time-varying parameters the electrochemical model becomes more representative of an aged battery cell. We show an improvement of the DFN model fidelity for aged cells that has the potential to extend the lifetime through optimized usage, and safer fast charging of the battery in future generations of BMS.

References

- [1] Xin Lai, Yuejiu Zheng, and Tao Sun. A comparative study of different equivalent circuit models for estimating state-of-charge of lithium-ion batteries. *Electrochimica Acta*, 259: 566–577, 2018. ISSN 0013-4686. doi: <https://doi.org/10.1016/j.electacta.2017.10.153>. URL <https://www.sciencedirect.com/science/article/pii/S0013468617322880>.
- [2] Xianke Lin, Kavian Khosravinia, Xiaosong Hu, Ju Li, and Wei Lu. Lithium plating mechanism, detection, and mitigation in lithium-ion batteries. *Progress in Energy and Combustion Science*, 87:100953, 2021. ISSN 0360-1285. doi: <https://doi.org/10.1016/j.pecs.2021.100953>. URL <https://www.sciencedirect.com/science/article/pii/S0360128521000514>.

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- [3] Valentin Sulzer, Scott G. Marquis, Robert Timms, Martin Robinson, and S. Jon Chapman. Python battery mathematical modelling (pybamm). *Journal of Open Research Software*, 9(1):14, 2021. doi: 10.5334/jors.309.
- [4] Simon EJ O’Kane, Weilong Ai, Ganesh Madabattula, Diego Alonso-Alvarez, Robert Timms, Valentin Sulzer, Jacqueline Sophie Edge, Billy Wu, Gregory J Offer, and Monica Marinescu. Lithium-ion battery degradation: how to model it. *Physical Chemistry Chemical Physics*, 24(13):7909–7922, 2022.