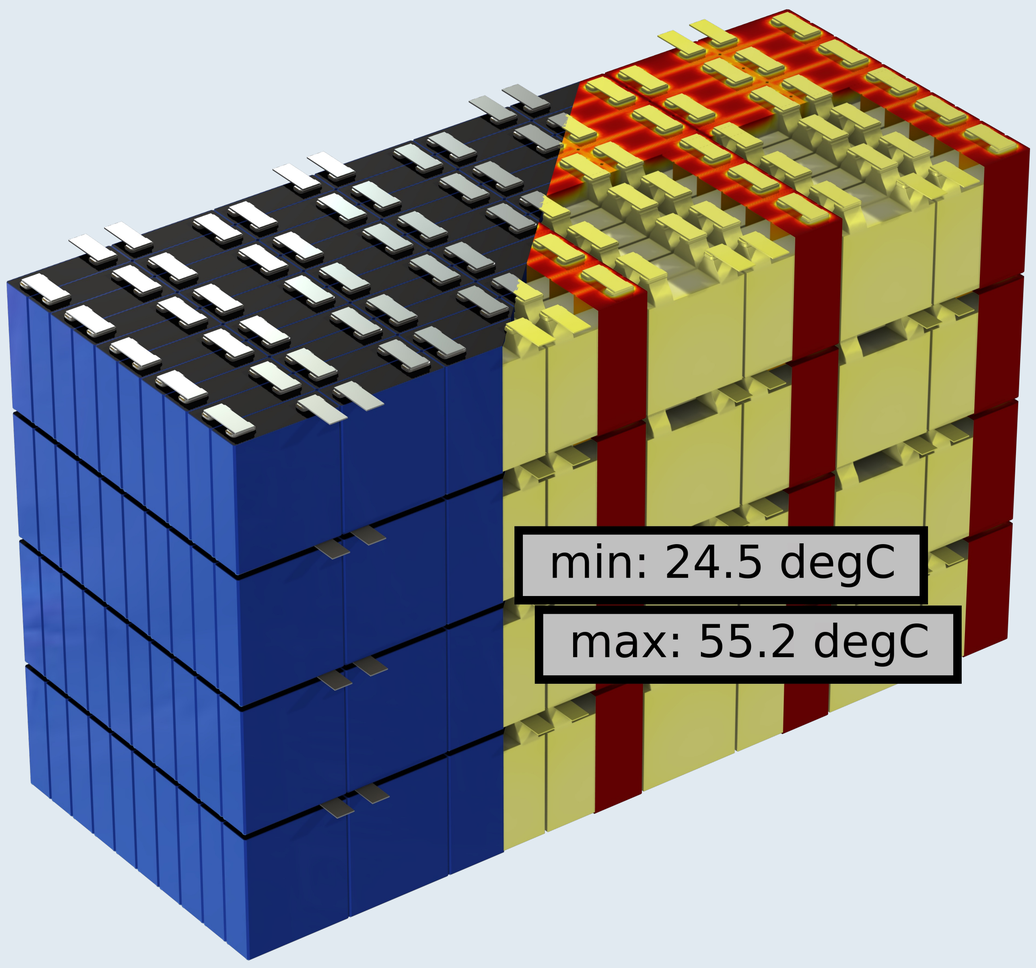

Novel Method For Predicting Lifetime Degradation Of Battery Packs Using COMSOL® Surrogate Models

Using the Deep Neural Network architecture that recently has been implemented in COMSOL®, we generate simulation results with a detailed chemistry model and used that as training, to scale up the battery modeling all the way up to entire pack simulations.

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Why it is necessary to go beyond traditional battery modeling

Battery modeling is traditional done either with 1D chemistry, constant degradation level, or even a lumped models. These methods do not accurately describe the battery, as they neglect the spatial dependence of the temperature. Temperature cascades into the complex transient dynamics with the current distribution, state of charge distribution, its effect on the chemical reaction kinetics, the local degradation density. They all freed back to uneven heat generation in a fully coupled and interconnected physic model. Taking these effects into account is no trivial matter, as it quickly becomes computationally too expensive to simulate the details. To overcome this issue while taking these effects into account, we use the Deep Neural Network feature implemented in COMSOL® to bride the gap between the large difference in scale between the microscopic diffusion in particles in the electrodes, and full pack with many cells.

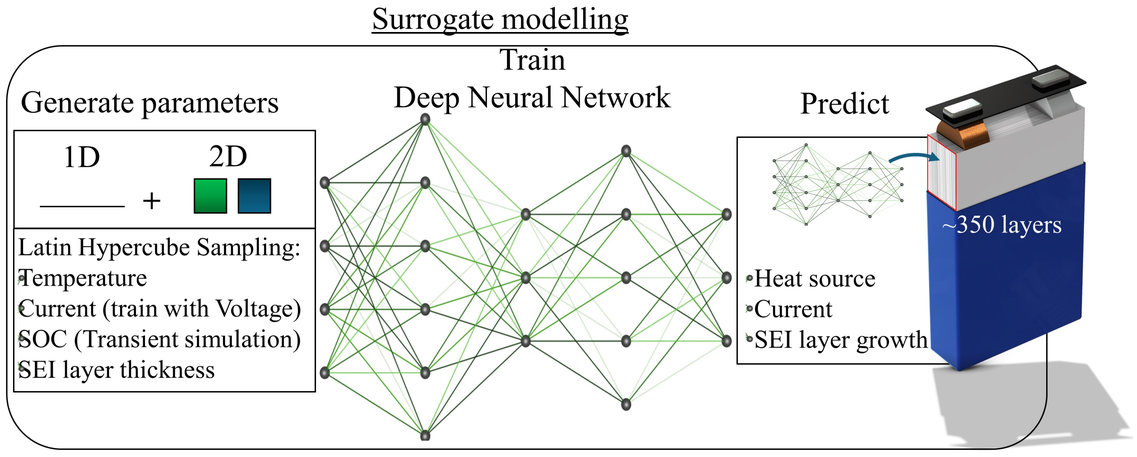

FIGURE 1. The procedure for generating data for, and training of, the Deep Neural Network used in the surrogate modeling.

Methodology for Surrogate Modeling

The Deep Neural Network provides a link between the chemistry modeling and the cell modeling. It does it by generating a dataset of all the relevant parameters by making a Latin Hypercube Sampling over relevant input parameters and recording relevant output parameters. That could be things such as the temperature, current, state of charge and SEI layer thickness as inputs, and the generated heat, voltage, and SEI layer growth as outputs. Having the dataset, it is then fed into a Neural Network with a sufficient topology for training it. Having this model, it now can predict the necessary outputs, based on simulation inputs, for homogenized chemistry layers in the cell. The important part is that it now couples back into the chemistry while calculating the fields that can only be described in 3D.

Simulating Multiphysics for Module

The efficiency of the method seen in figure 1, allows for fast calculation of battery cells and modules. This gives the possibility of calculating the temperature field integrated up in full 3D, with proper boundary conditions and with cooling flow as well as volumetric heat from joule heating from the current and chemistry. This is seen on figure 2. The uneven temperature this results in, gives uneven chemical overpotential, and therefore uneven state of charge, with a dynamic Solid Electrolyte Interface (SEI) which represents the degradation we are using to calculate the state of health of the battery module. This can then be used as the initial condition when calculating the next charging or discharging, which therefore will compound on the degradation.

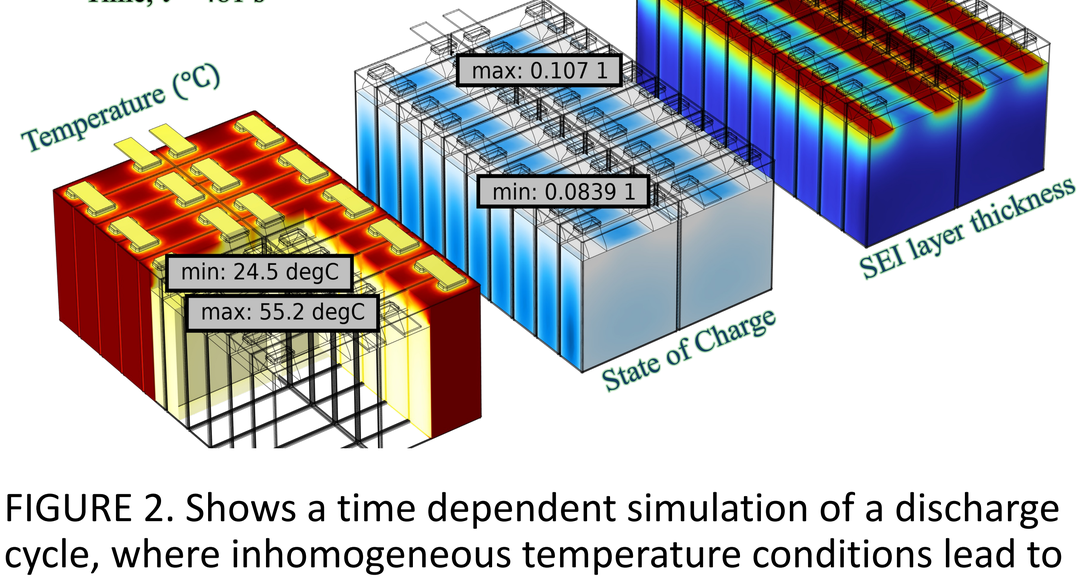

FIGURE 2. Shows a time dependent simulation of a discharge cycle, where inhomogeneous temperature conditions lead to uneven state of charge and degradation in terms of SEI layer.

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