

Uncertainty Assessment and Sensitivity Analysis of Heat Generation within a Lithium-Ion Battery

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Introduction

Dedicated work in modeling, simulation and design optimization of Lithium-ion Battery (LIBs) was done in the past decades, and still, the most widely used one for electrochemical processes is the Newman model.^[1] The underlying parameters are treated deterministically, but the impact of uncertainty due to experimental accuracy limitations and cell-to-cell variations have a significant impact on battery performance.^[2] In this approach the analysis of uncertainty related to heat generation is the major focus due to its impact on safety and battery performance at a systems level.

At DLR VE a P2D-3D electrochemical-thermal battery model is established^[3] and used in order to simulate the deterministic behaviour of a virtually represented commercial lithium-ion pouch battery cell.

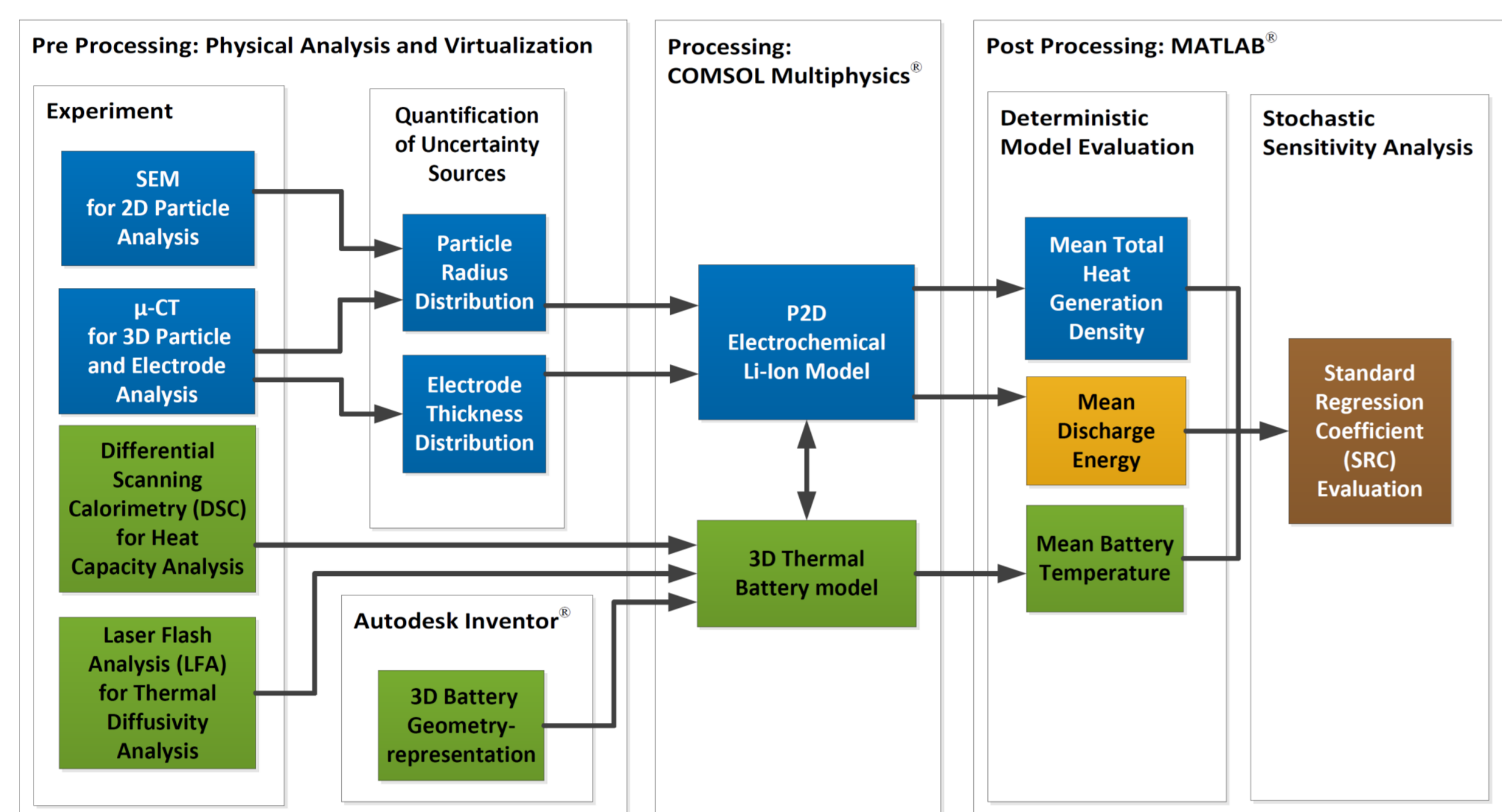


Fig. 1: Classification of methods and quantities for the battery model analysis

Uncertainty Assessment of Battery Parameters

Uncertainties and inhomogeneities of the electrochemical submodel are mainly hidden within the electrochemical parameters and geometric interface relations of the cell materials.

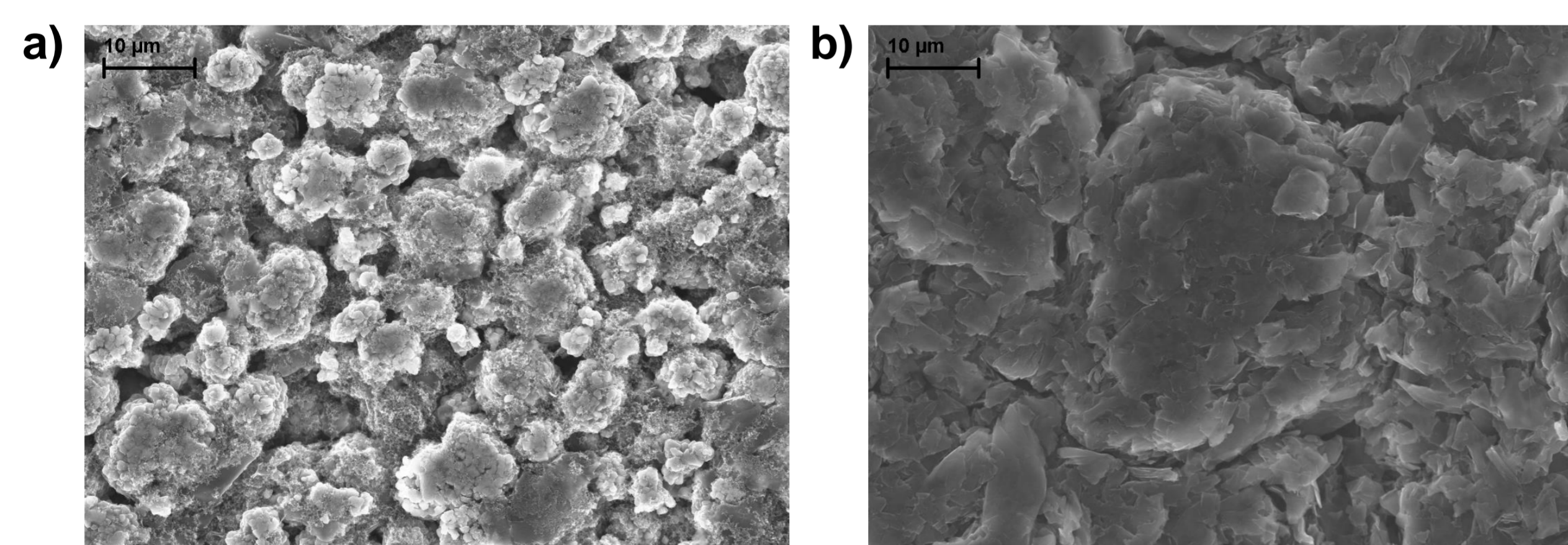


Fig. 2: SEM Images of a) the positive NMC and b) the negative graphite electrode; an InLens electron detector with an accelerator voltage of 20 kV was used.

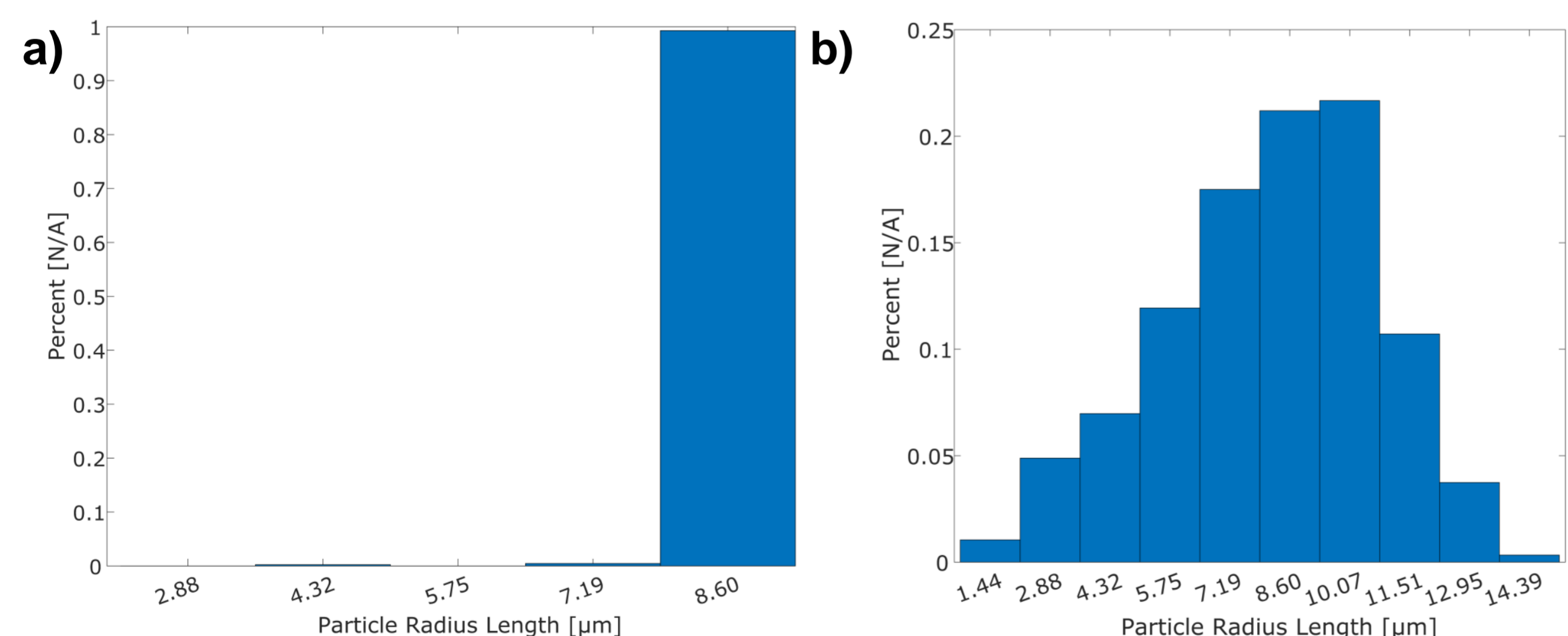


Fig. 3: μ -CT 2D particle volume analysis of a) the positive NMC with porous electrode thickness $L_{pos} = 42,10 \pm 0,95 [\mu m]$ and b) the negative graphite electrode with porous electrode thickness $L_{neg} = 59,47 \pm 1,05 [\mu m]$ to determine the particle radius distribution.

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Deterministic: Battery Model

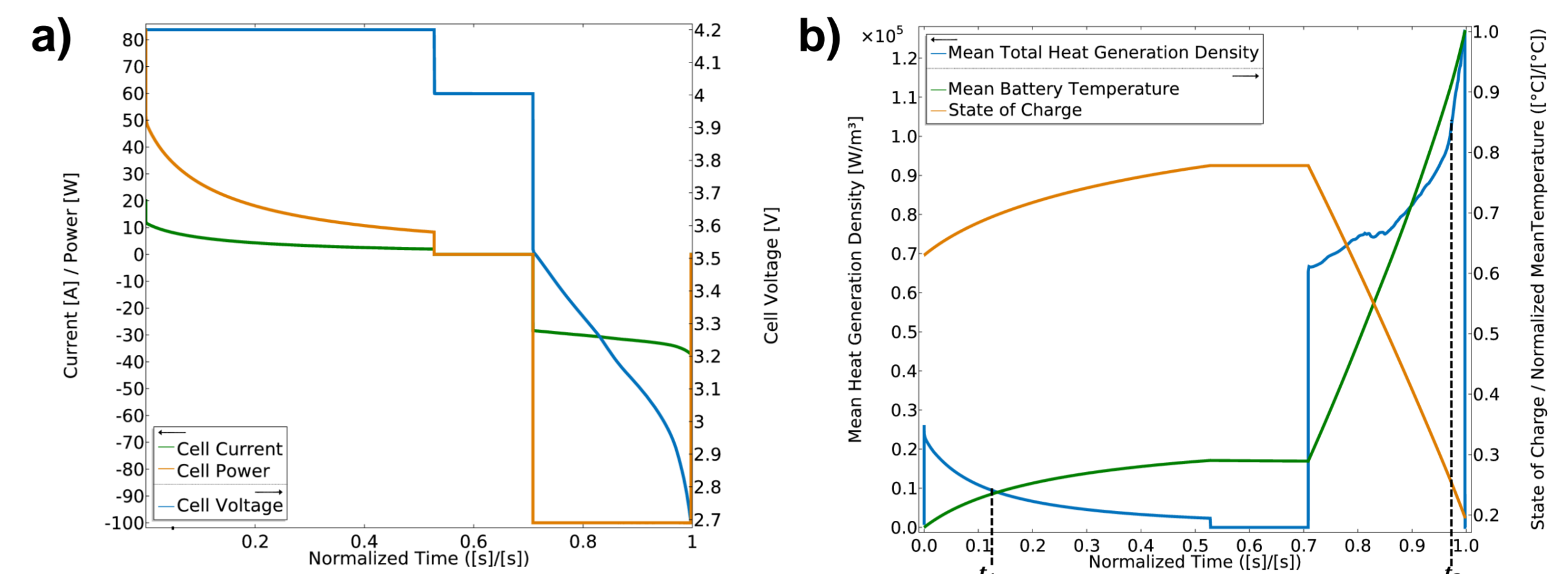


Fig. 4: a) Simulated cell performance profiles of CV-charge, rest phase and CP-discharge-cycle as a function of normalized time
b) Simulated quantities of interest: Mean total heat generation density, mean battery temperature and state of charge as a function of normalized time

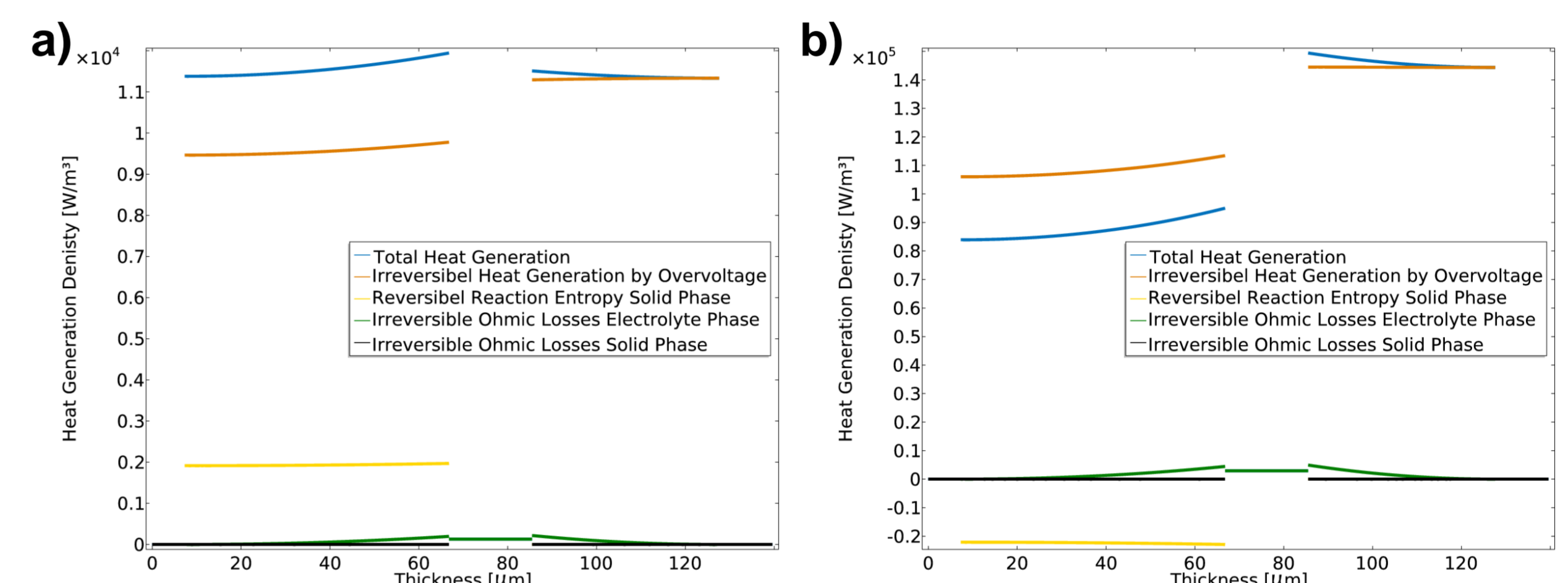


Fig. 5: a) Simulated partial and total heat generation density as a function of cell thickness at time t_1 during charge-phase
b) Simulated partial and total heat generation density as a function of cell thickness at time t_2 during discharge-phase

Stochastic: Sensitivity Analysis

The measure of sensitivity^[4] of the model response $Y = \{Y_1, \dots, Y_3\}$ to each input variable $X = \{X_1, \dots, X_4\}$ is given by the standard regression coefficients (SRC); β least-squares coefficients, $M = 4$, $A = [X_1, \dots, X_4]$ parameter matrix, $\hat{\beta}$ least-squares coefficients estimator, $y \in Y$, σ_i standard deviation of the input sample X_i and σ_y being total standard deviation of Y :

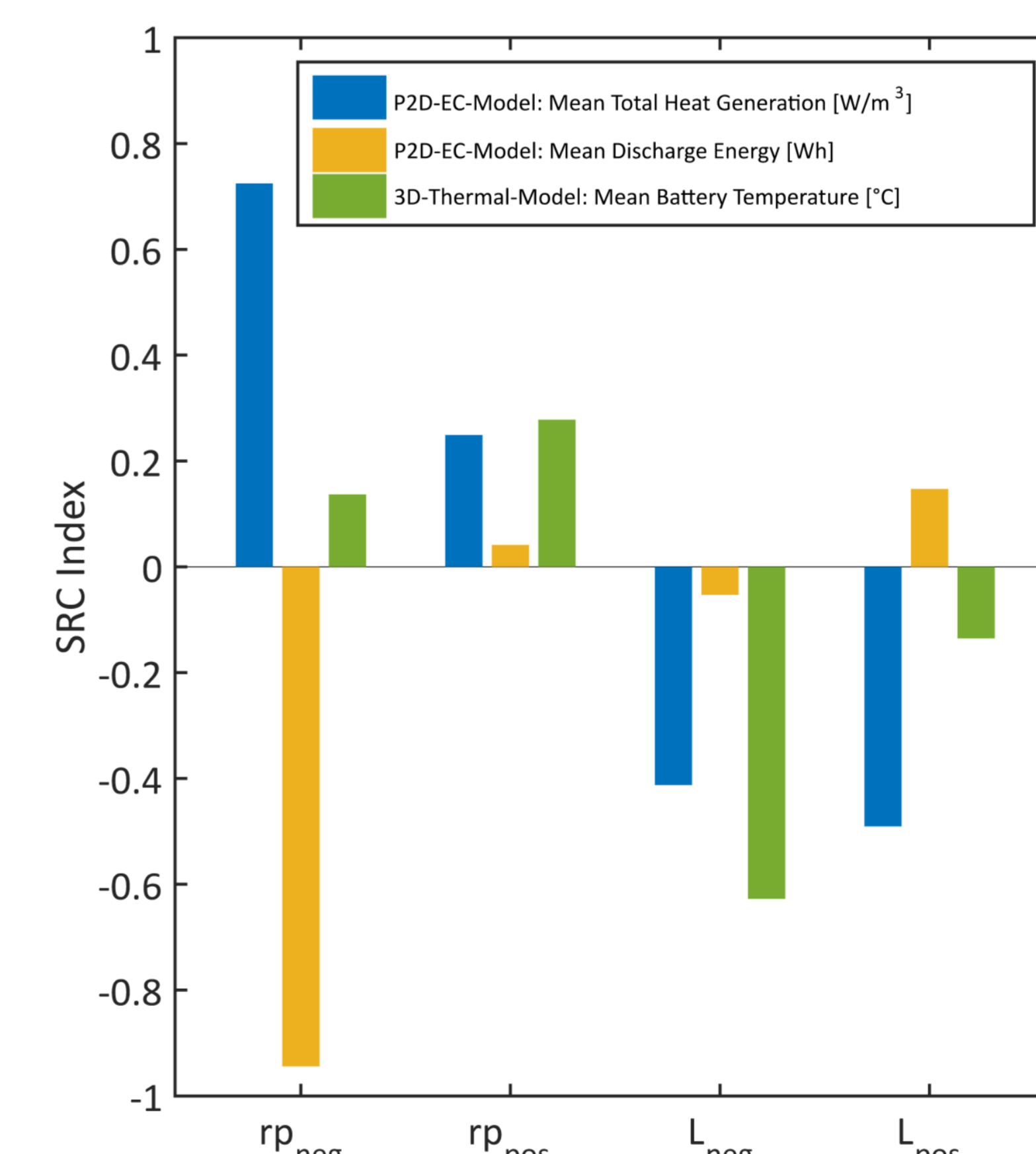


Fig. 6: SRC Index as a bar chart of input parameter selection: negative porous electrode particle radius rp_{neg} , positive porous electrode particle radius rp_{pos} , negative porous electrode thickness L_{neg} and positive porous electrode thickness L_{pos}

Linear Regression:

$$Y \approx \beta_0 + \sum_{i=1}^M \beta_i X_i$$

Coefficient Estimation:

$$\hat{\beta} = (A^T A)^{-1} A^T y$$

$$SRC_i = \frac{\hat{\beta}_i \sigma_i}{\sigma_y}$$

Significant Tendencies (≥ 0.5):

$$rp_{neg} \uparrow: E \downarrow, H \uparrow$$

$$L_{neg} \uparrow: T \downarrow$$

$$L_{pos} \uparrow: H \downarrow$$

Conclusion

Uncertainty of material parameters of a LIB cell model has a big influence on the battery performance. Therefore, a new test setup was developed to propose uncertainty distribution of input parameters, predict the impact of uncertainty for battery performance and derive accurate behaviour of the quantities of interest: heat generation, mean discharge energy and mean battery temperature. We will further utilize the model for comparative studies of commercial cell variants.

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