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Identification of Relevant Parameters for Battery Model using Calibration Under Discharge Condition

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Motivation

- Energy turnaround
  - E-mobility awareness increases
  - Alternative energy sources

    → more and more energy storages are needed

- Weaknesses of energy storages
  - Thermal Runaway
  - Decreasing capacity
  - Small energy density

→Understand charge and mass transport of batteries before production

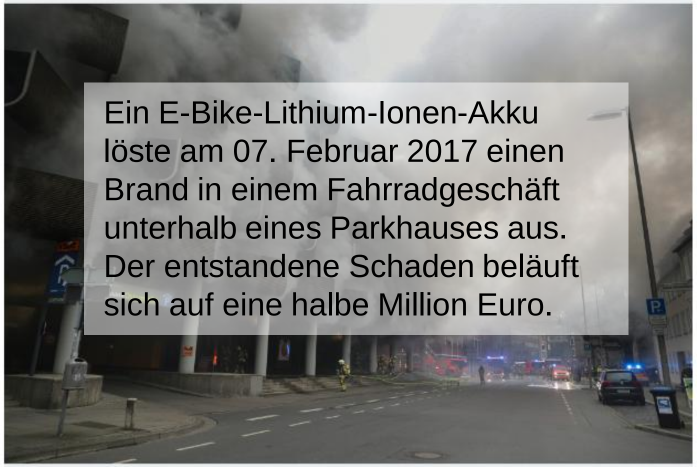
→Simulation of batteries beyond known limits

9. Oktober 2016, 18:57 Uhr Brennende Akkus

Schwelendes Verfahren

Das verschmorte Handy aus dem Flugzeug der Southwest Airlines. (Foto: Brian Green/Reuters)

Quelle: www.sueddeutsche.de



Quelle: www.all-electronics.de

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Battery Simulation

Simulation Task – Identification and Calibration

- Newman Model based (LIBERA Project from CADFEM/THI)
  - **Lithium-Ion Diffusion**
  - **Charge transport**
  - **Electrochemical reaction**

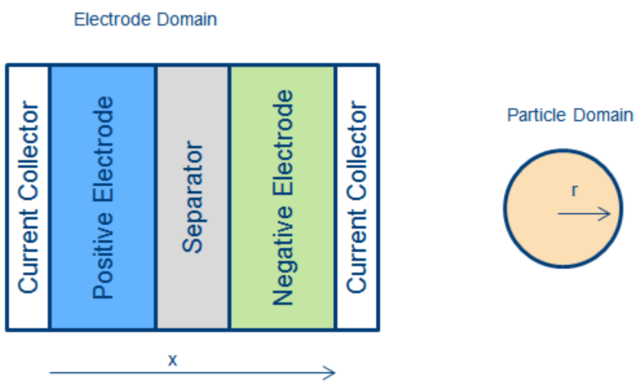
- Pseudo **2D**-Model:

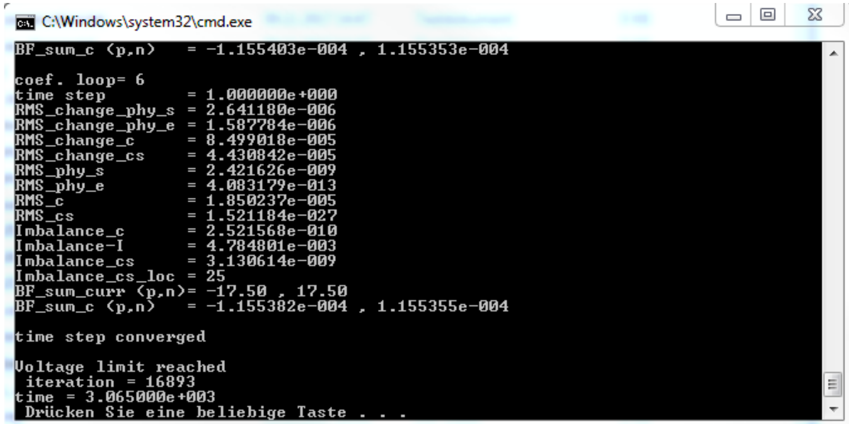
  Dimension x:
  transport from negative to positive electrode

  Dimension r: particles describing porosity of electrodes

  Main Output signal: e. g. Voltage vs. charge

- Goal:
  - Identify driving parameters
  - Calibrate signals between simulation and test

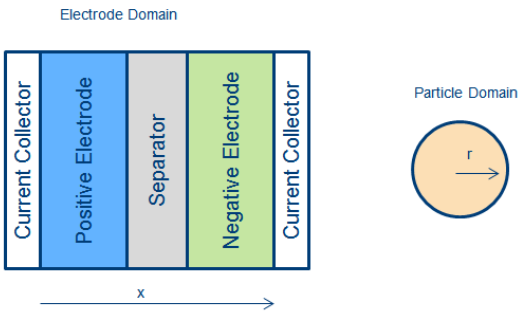


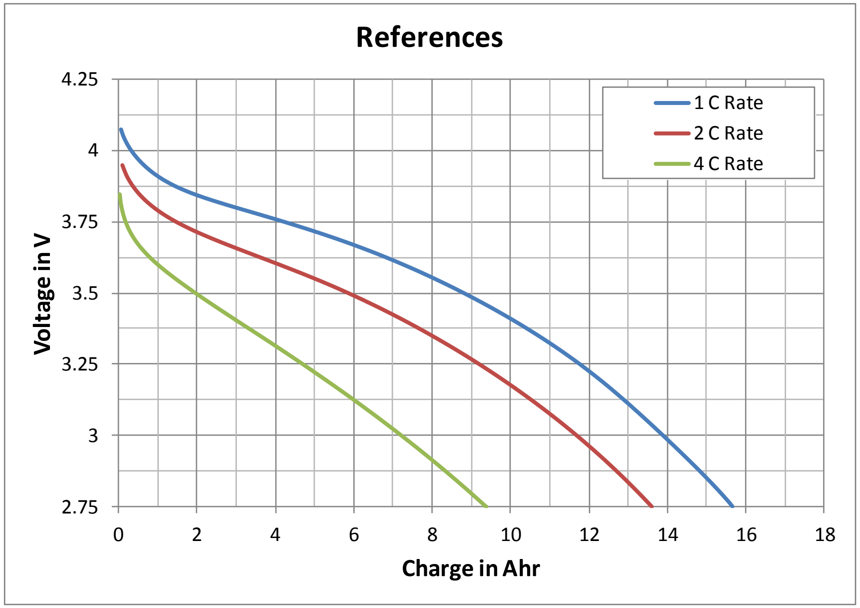


Parametric Workflow for Battery Simulation

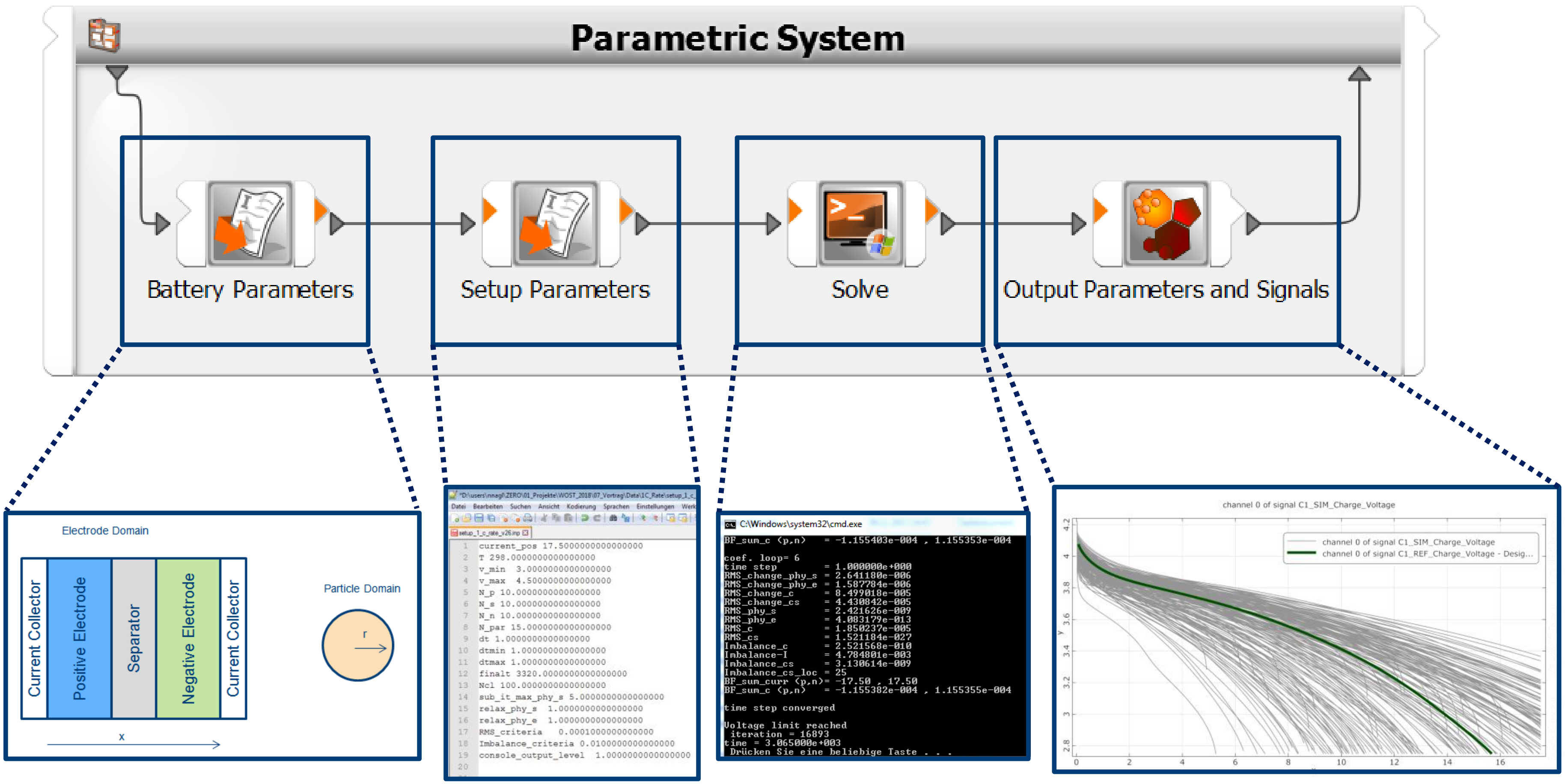
- Battery simulation on electrode level
- Input parameters
  - Physical battery model parameters
  - Setup parameters
- Output parameters
  - Voltage vs. time
  - Current vs. time

- Reference Signals
  - 1 C Rate Voltage vs. Charge
  - 2 C Rate Voltage vs. Charge
  - 4 C Rate Voltage vs. Charge





Parametric Workflow for Battery Simulation

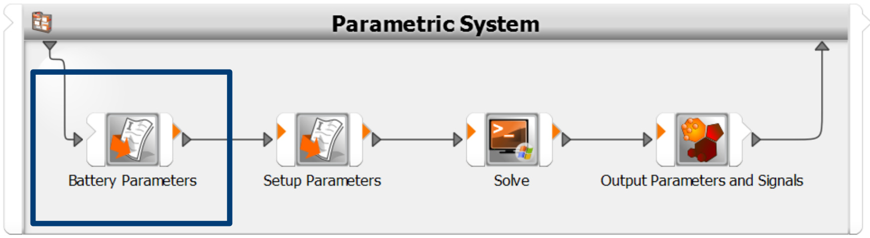


Battery Parameters and Ranges for Sensitivity Analysis

- 13 Input Parameter

- Which parameters influence the discharge signal?

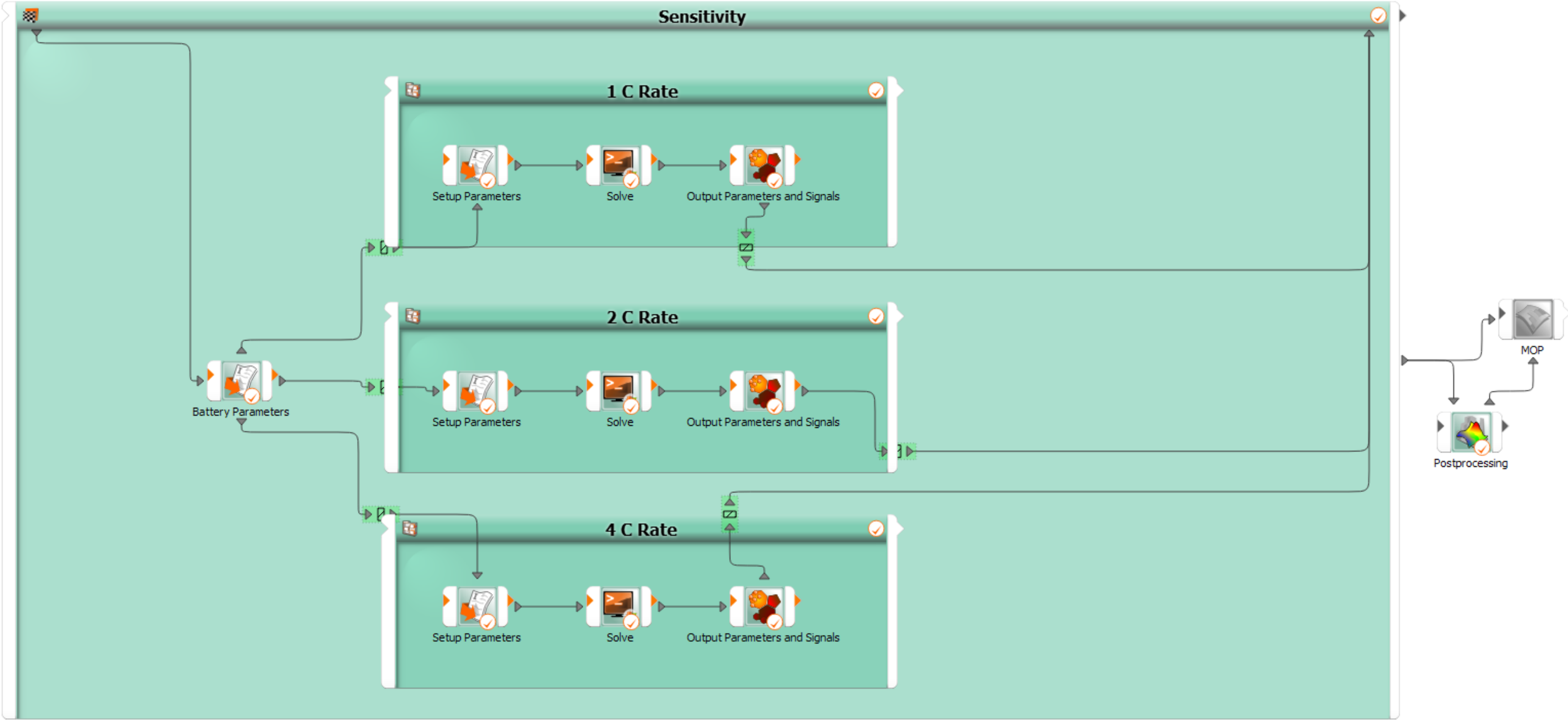
→ Sensitivity analysis



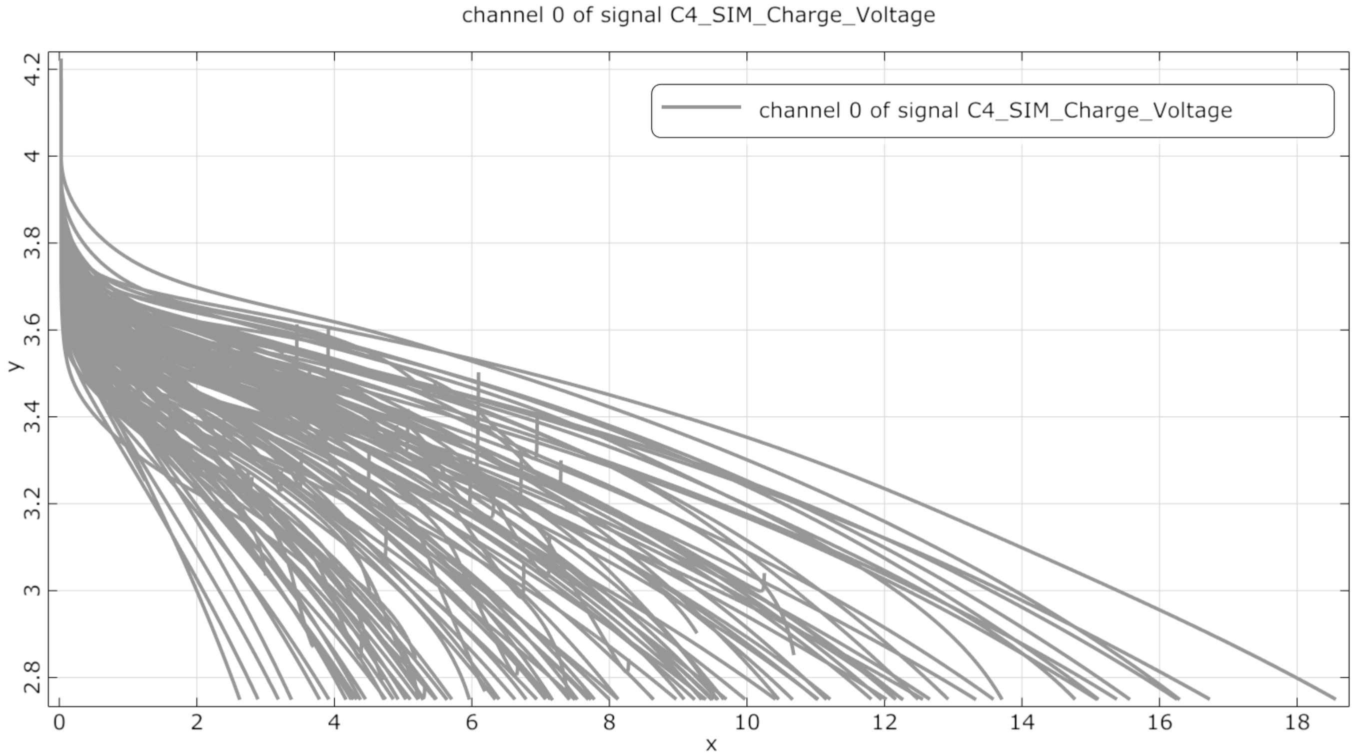
Name	Description	Unit	Reference Value	Lower Bound	Upper Bound
D_e	electrolyte phase Li-ion diffusion coefficient	m^2/s	7.50E-11	3.00E-11	1.20E-10
Ds_n	diffusion coefficient at the solid phase. negative electrode	m^2/s	3.90E-14	1.56E-14	6.24E-14
Ds_p	diffusion coefficient at the solid phase. positive electrode	m^2/s	1.00E-13	4.00E-14	1.60E-13
ep_n	volume fraction of electrolyte at the negative electrode	-	0.357	0.143	0.571
ep_p	volume fraction of electrolyte at the positive electrode	-	0.444	0.266	0.622
epf_n	volume fraction of filler material at the negative electrode	-	0.172	0.103	0.241
epf_p	volume fraction of filler material at the positive electrode	-	0.259	0.104	0.414
k_n_ref	electrochemical reaction rate constant of negative electrode	$mol/m^2/s/(mol/m^3)^{1.5}$	2.33E-11	9.32E-12	3.37E-11
k_p_ref	electrochemical reaction rate constant of positive electrode	$mol/m^2/s/(mol/m^3)^{1.5}$	2.33E-11	9.32E-12	3.73E-11
Rs_n	particle radius in negative electrode	m	1.25E-05	5.00E-06	2.00E-05
Rs_p	particle radius in positive electrode	m	8.00E-06	3.20E-06	1.28E-05
sigma_n	electrical conductivity of negative electrode	S/m	100	90	110
sigma_p	electrical conductivity of positive electrode	S/m	3.80	3.42	4.18

Simultaneous Simulation Workflow for all 3 C-Rates

- Sensitivity analysis with 200 designs



Characterization of Calculated Signals



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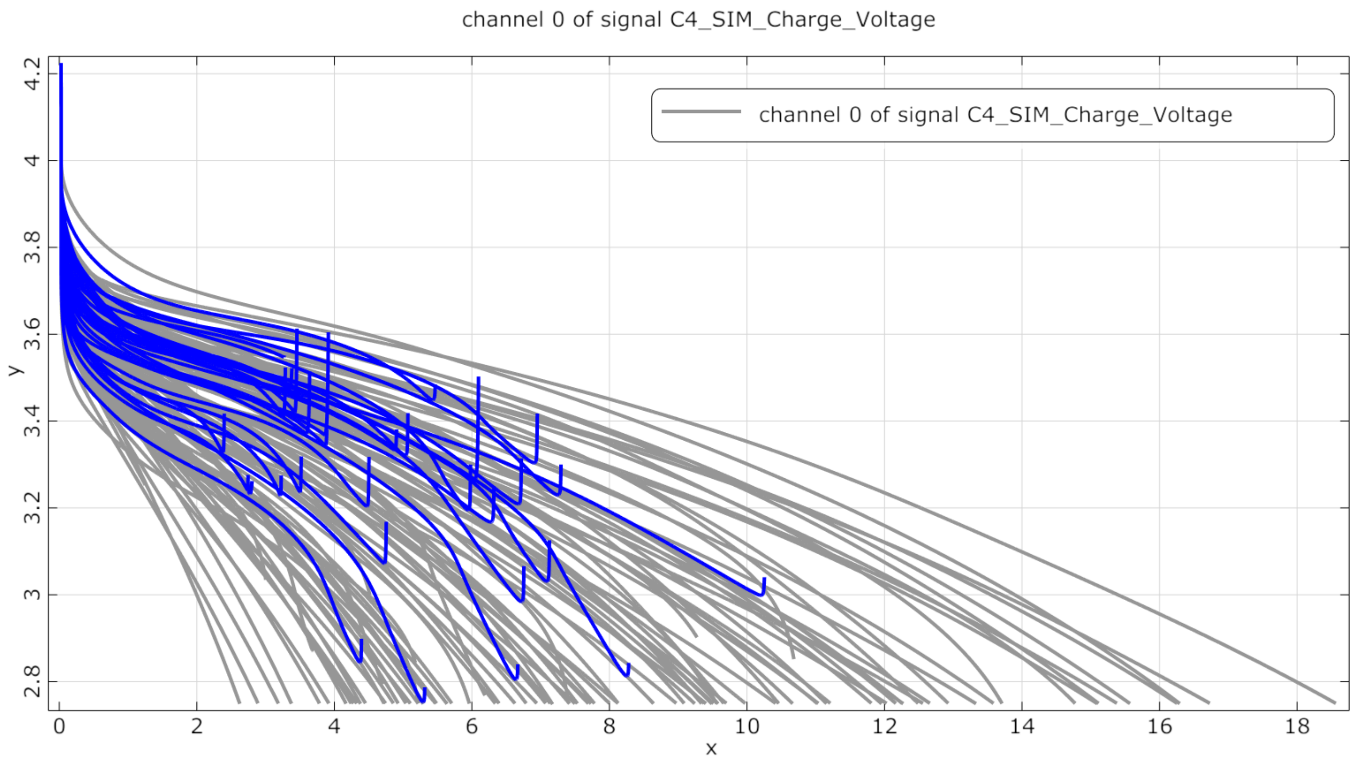
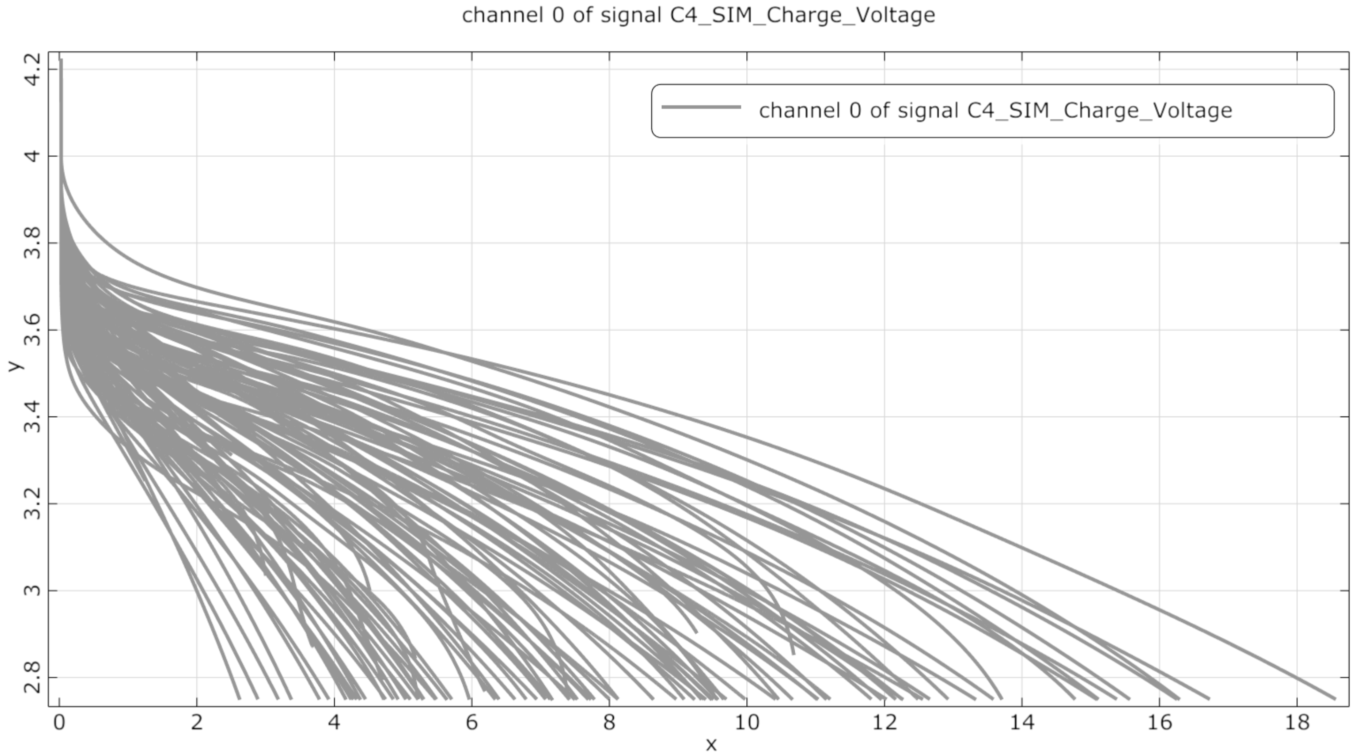
Characterization of Calculated Signals



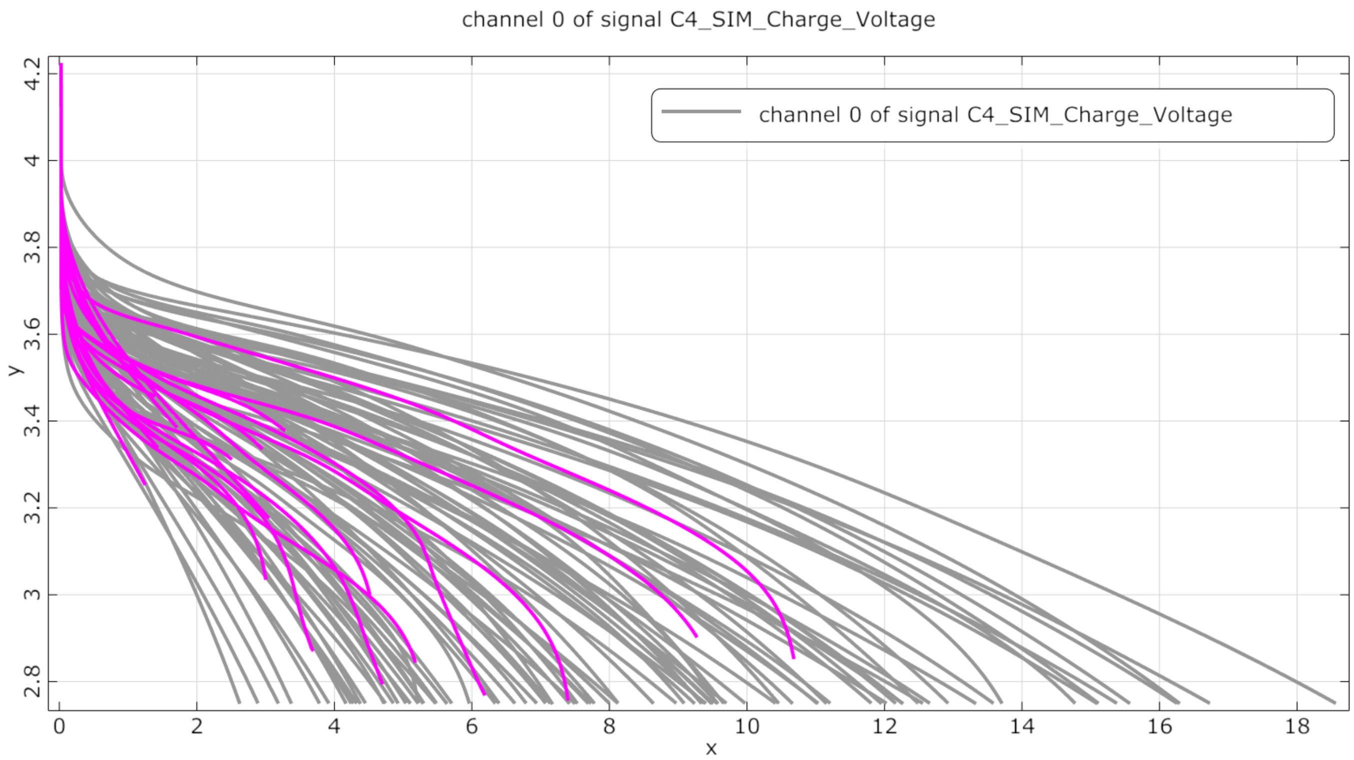
- Non-physical convergence problems → unconverged solution
- New check output parameter: if converged then 0 otherwise -1

Characterization of Calculated Signals



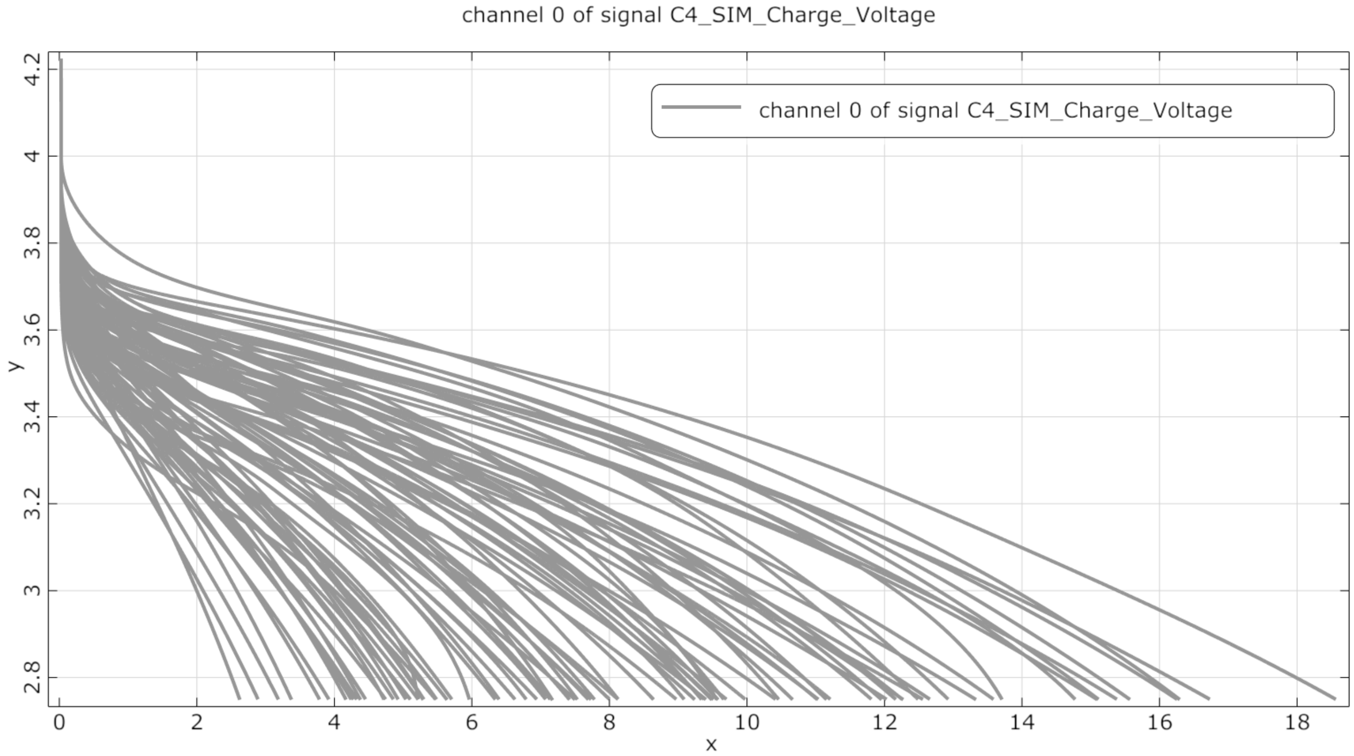
- Unconverged Signals are neglected

Characterization of Calculated Signals



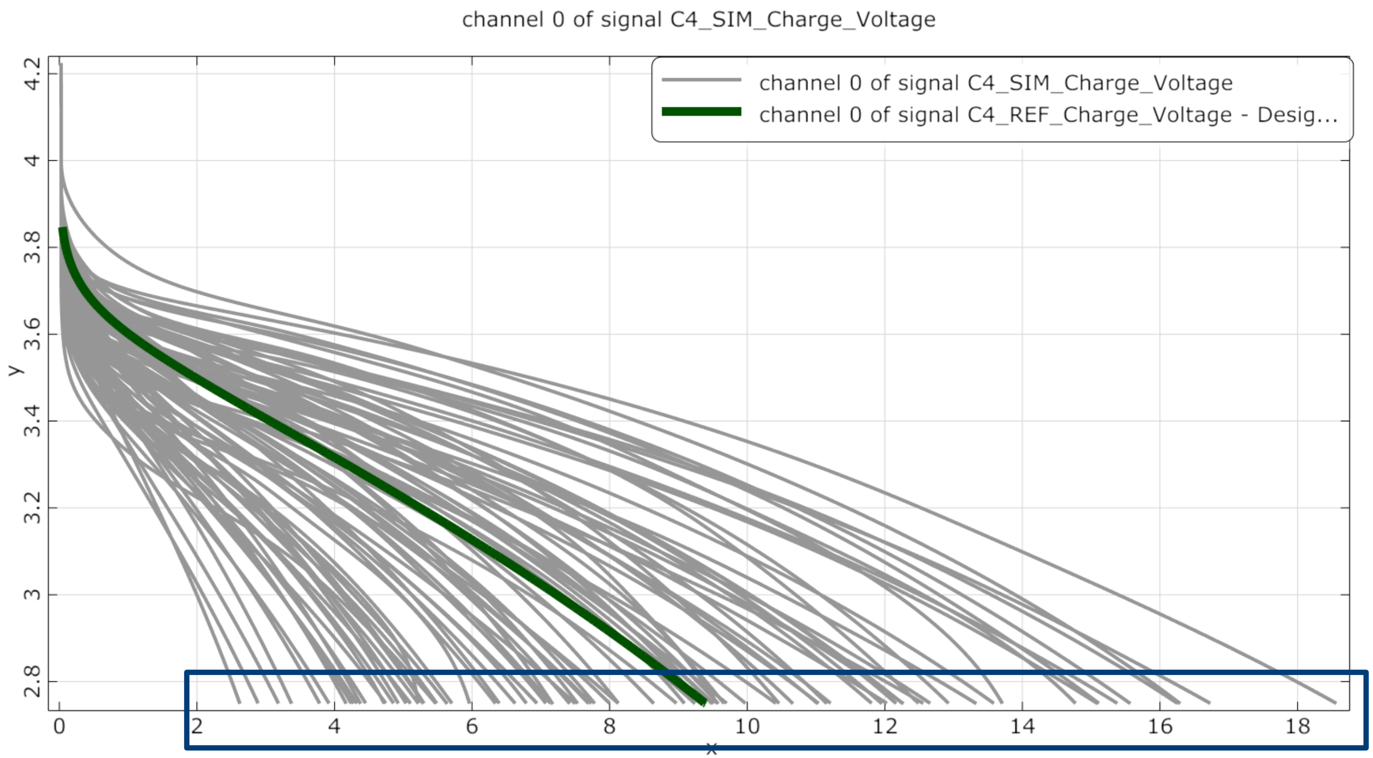
- Limit of 2.75 V is not reached
- Additional check output parameter: if limit reached then 0 otherwise -1

Characterization of Calculated Signals



- Limit of 2.75 V is not reached
- Signals are neglected

Characterization of Calculated Signals

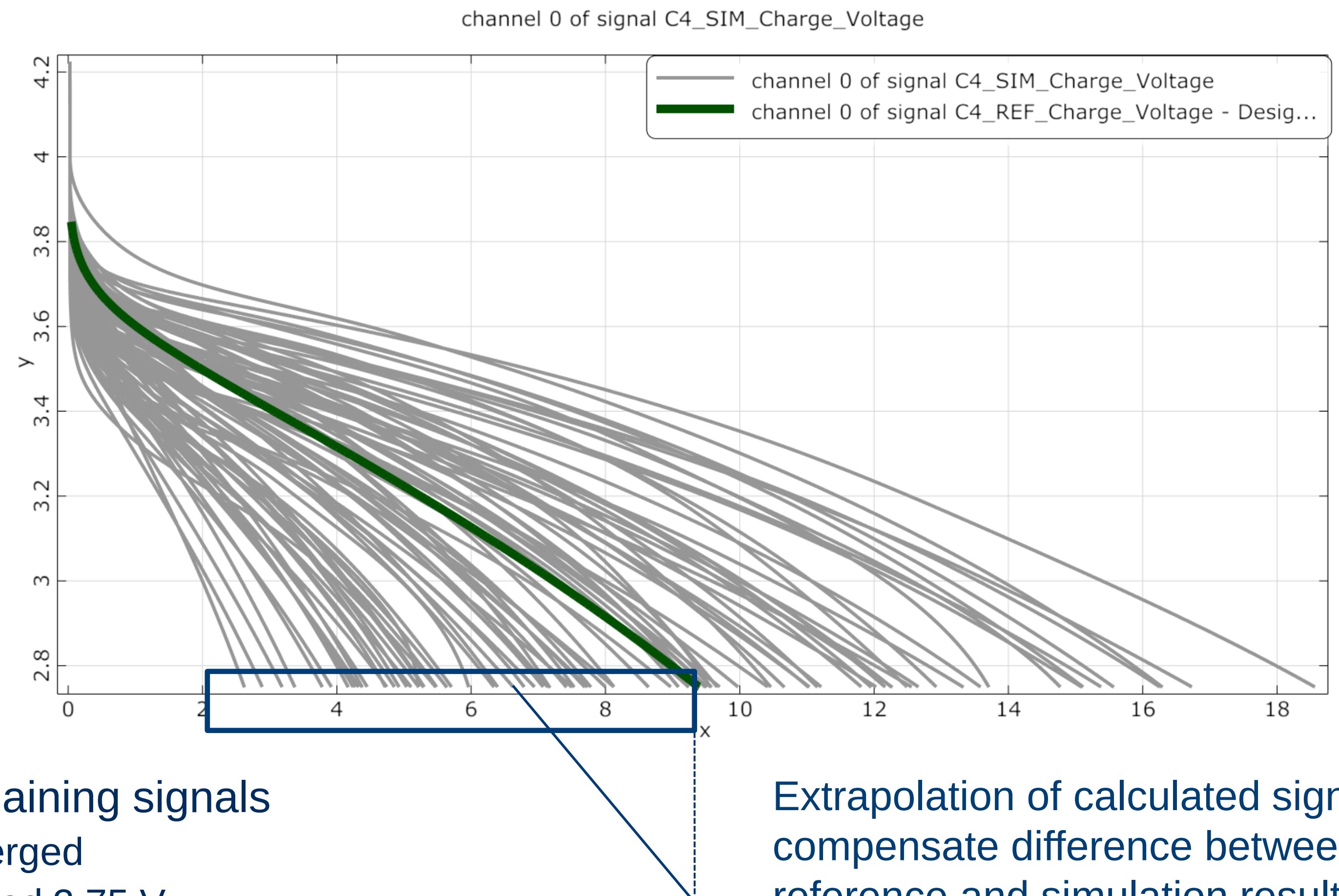


- All remaining signals
  - converged
  - reached 2.75 V
  - Both check output parameters = 0

BUT

Signal lengths differ!

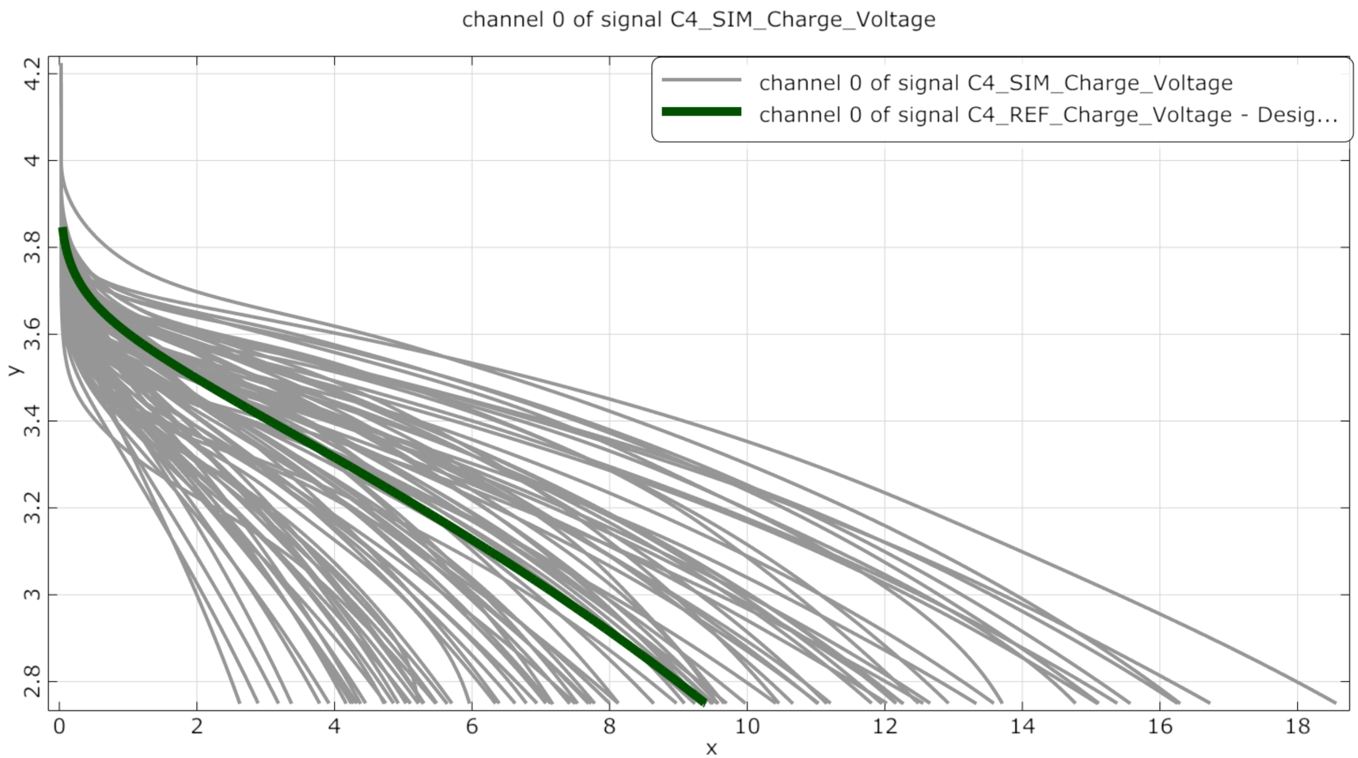
Characterization of Calculated Signals



- All remaining signals
  - converged
  - reached 2.75 V

Extrapolation of calculated signal to compensate difference between reference and simulation result?

Characterization of Calculated Signals

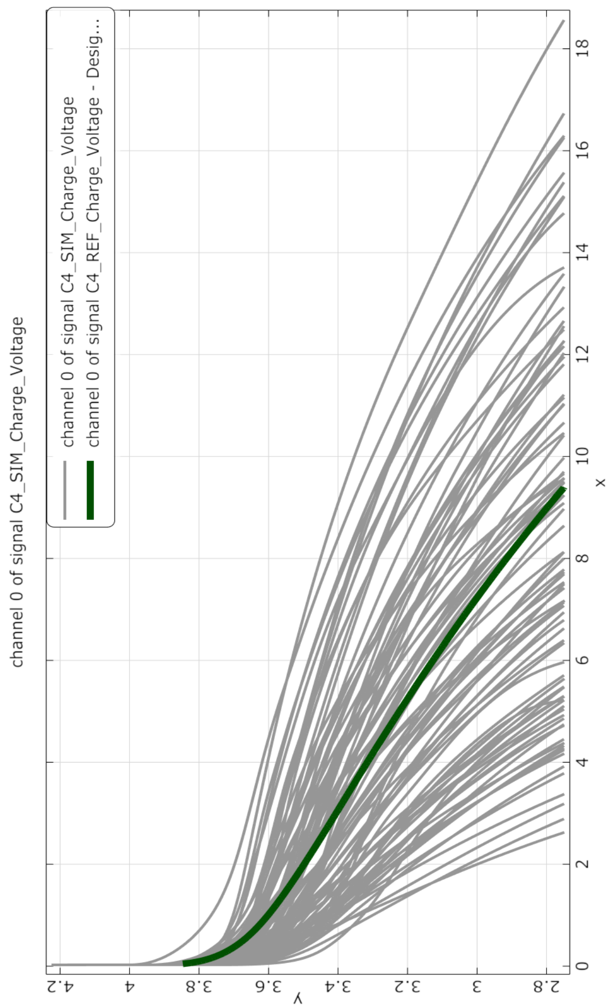


- All remaining signals
  - converged
  - reached 2.75 V

Extrapolation is NO option!

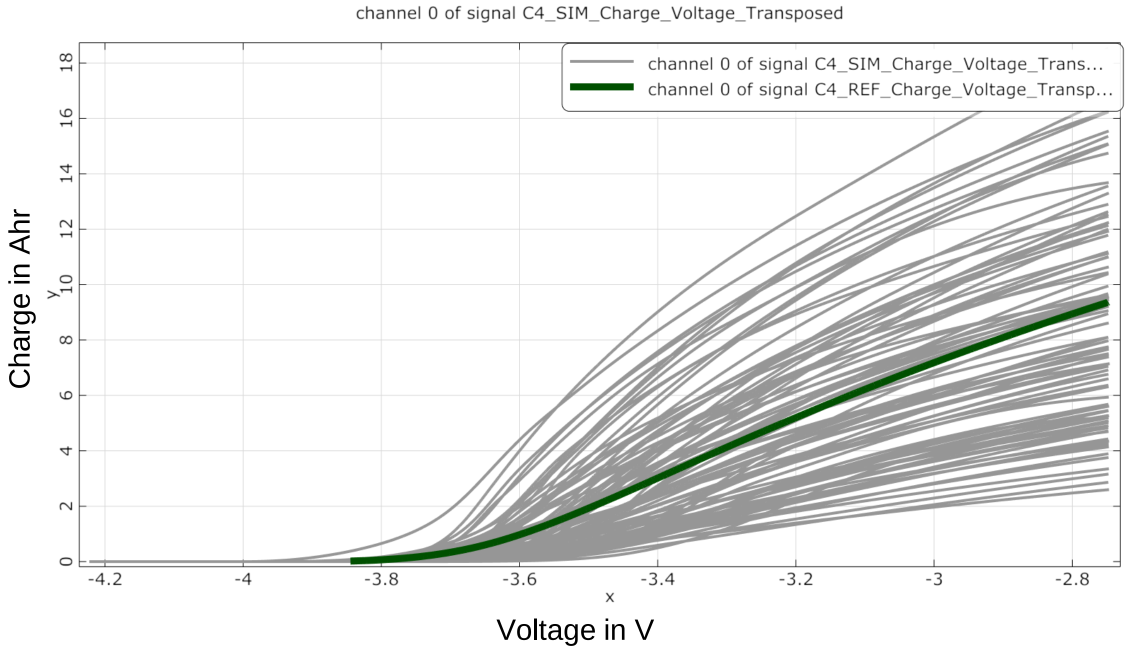
There is a solution for this problem!

Characterization of Calculated Signals



Characterization of Calculated Signals

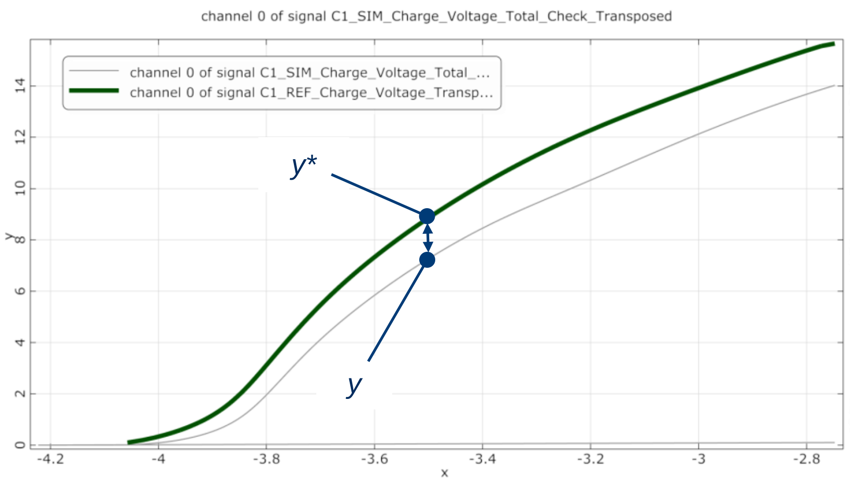
- Transpose signal
- All signals have same length
- No extrapolation – raw data from simulation
- Calibration possible



Calibration – Minimize Difference between Reference and Simulation

- Root Mean Squared Error RMSE (normalized) ≙ Difference

$$RMSE = \sigma_\epsilon = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i^* - y_i)^2}$$

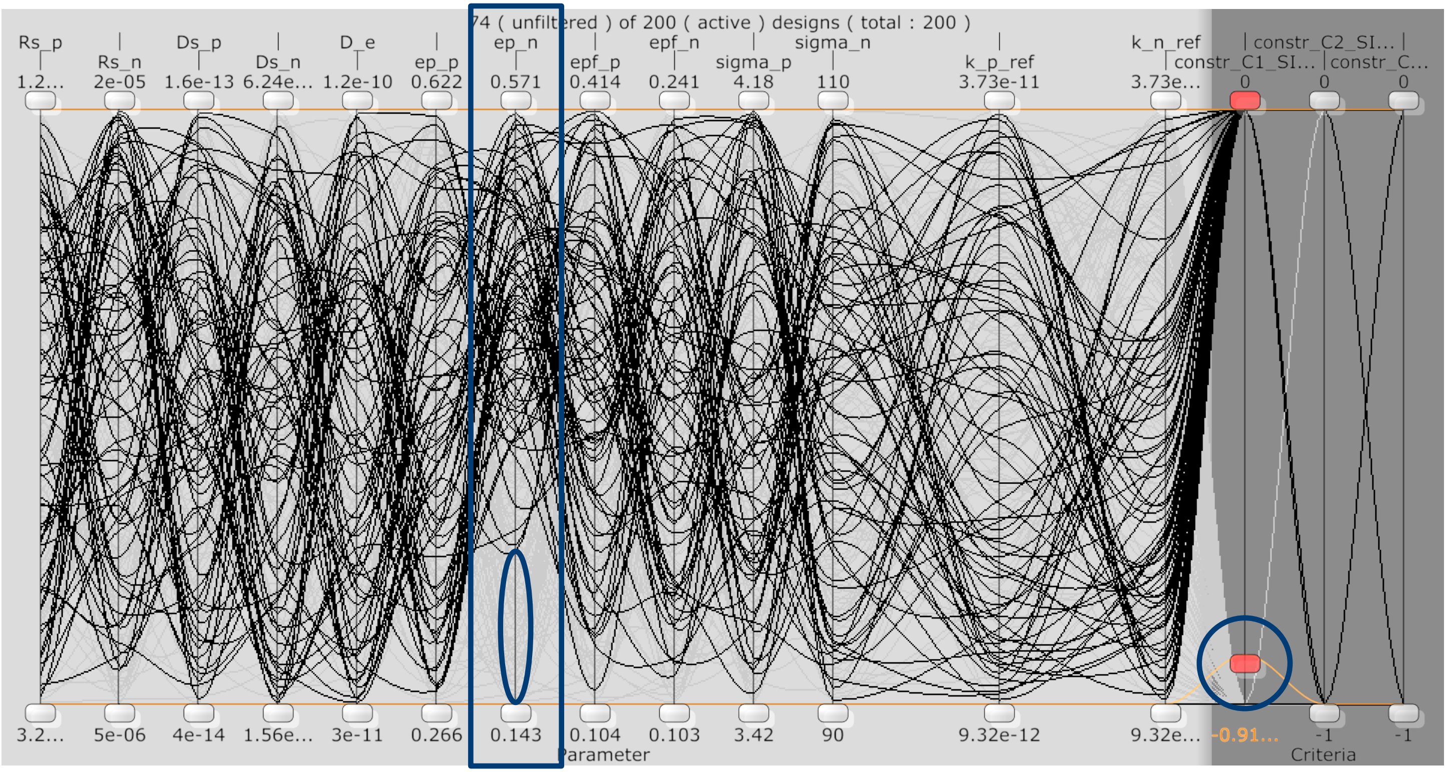


- *n*: Number of data points
- *y**: Reference value (measurement)
- *y*: Calculated value (battery simulation)

→ Optimization task: Minimizing the difference for all necessary data points

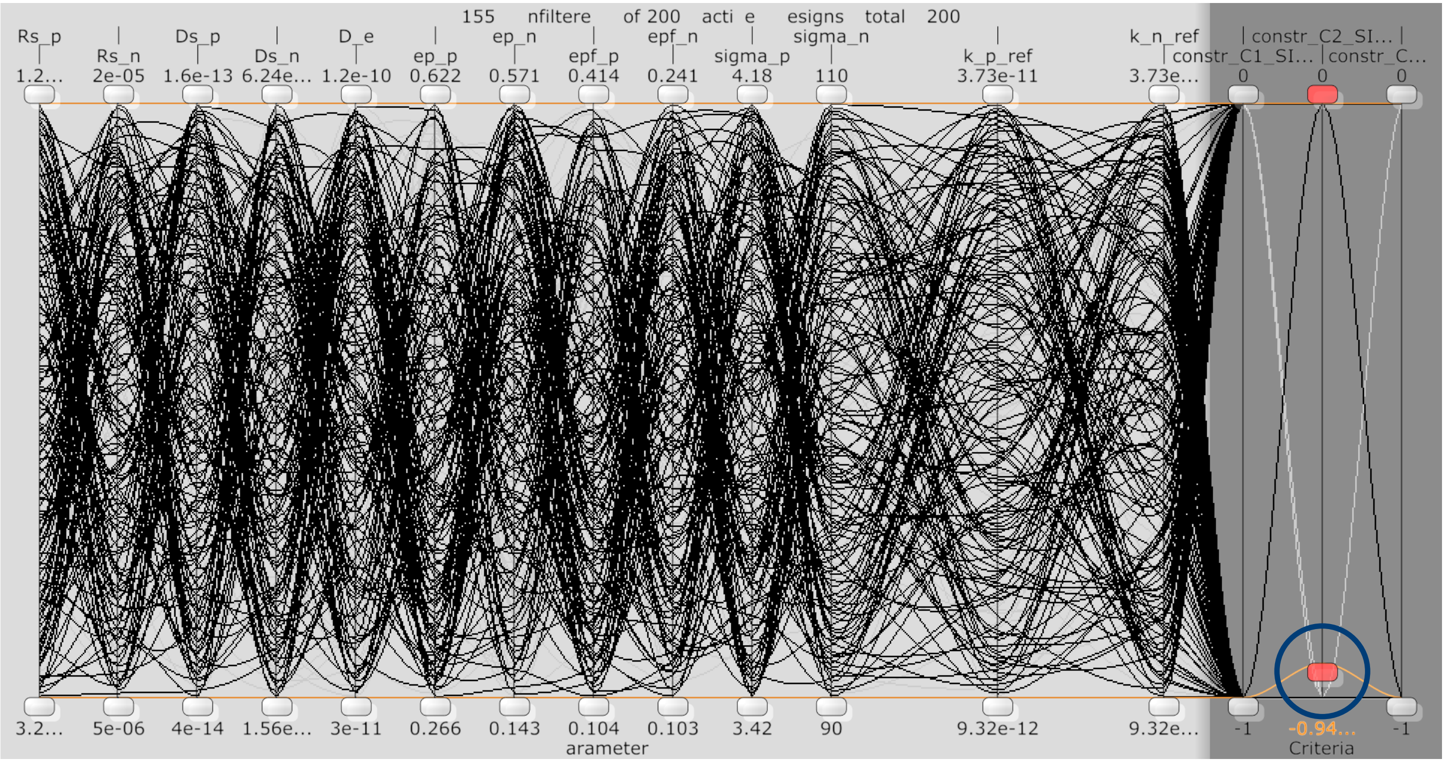
Identification of non-valid Designs

- Parallel Coordinates Plot
  - Designs for check output parameter 1 C rate = -1 are deselected



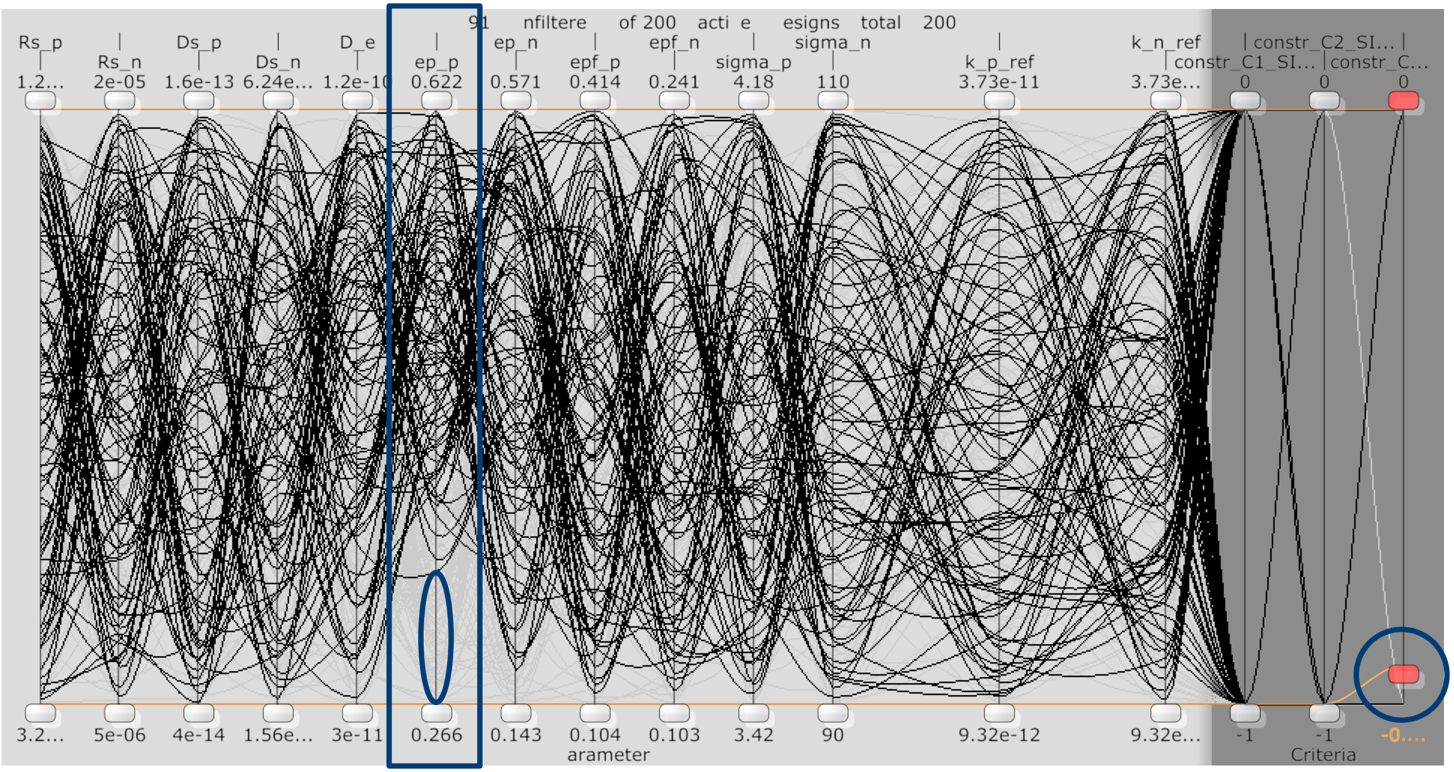
Identification of non-valid Designs

- Parallel Coordinates Plot
  - Designs for check output parameter 2 C rate = -1 are deselected



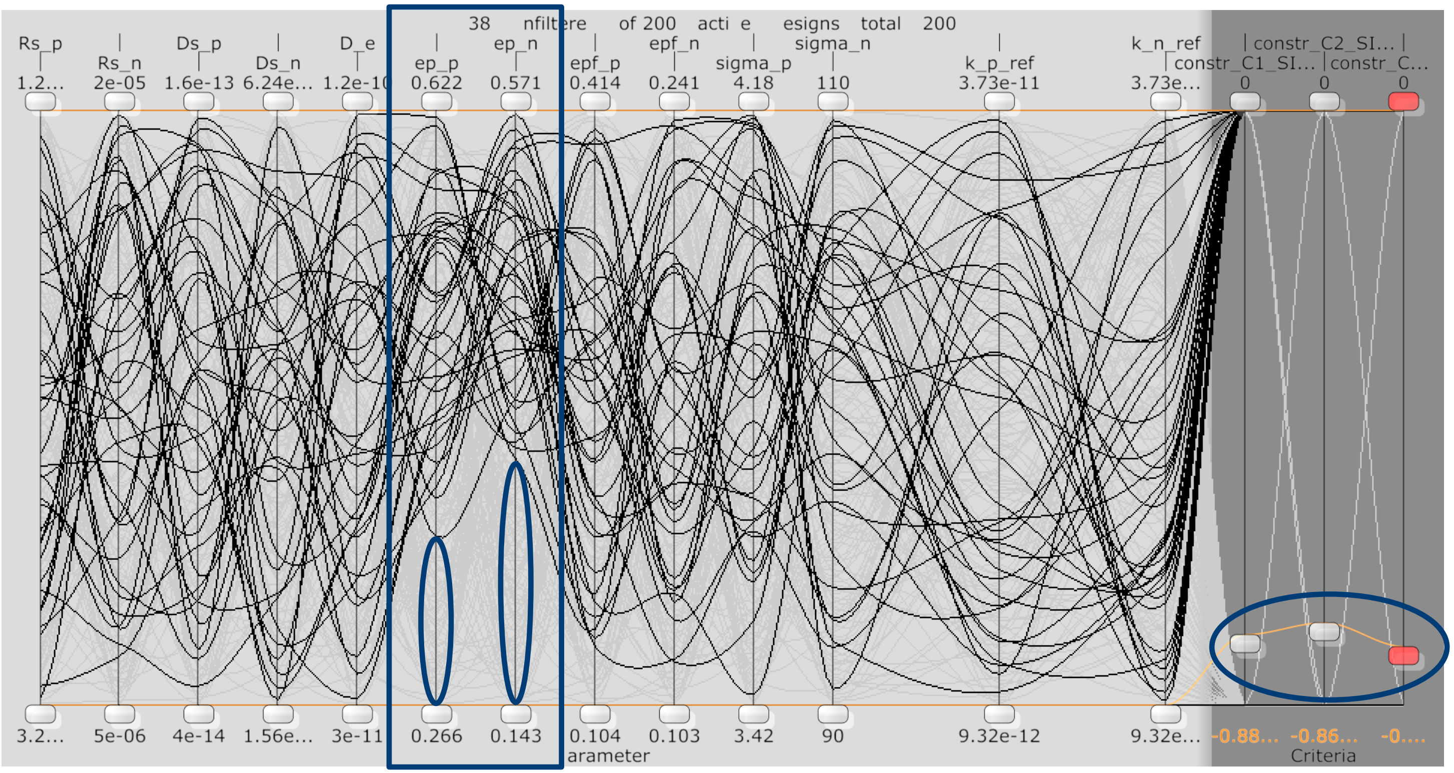
Identification of non-valid Designs

- Parallel Coordinates Plot
  - Designs for check output parameter 4 C rate = -1 are deselected



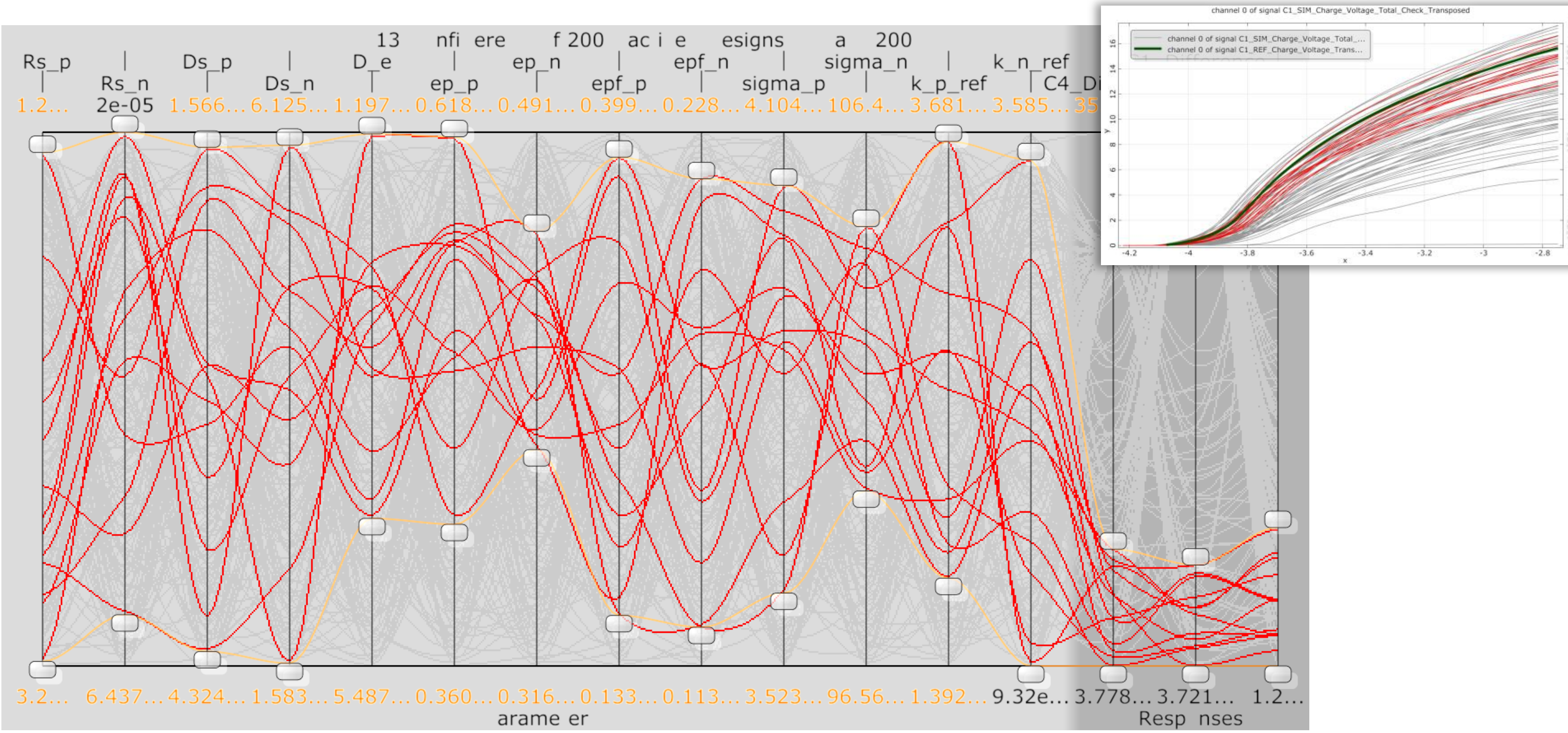
Identification of non-valid Designs

- Parallel Coordinates Plot
  - Designs for check output parameter for all C rates = -1 are deselected



Identification of non-valid Designs

- Parallel Coordinates Plot
  - Select designs with low difference values → new lower and upper bounds



2^{nd} Sensitivity with Reduced Parameter Bounds

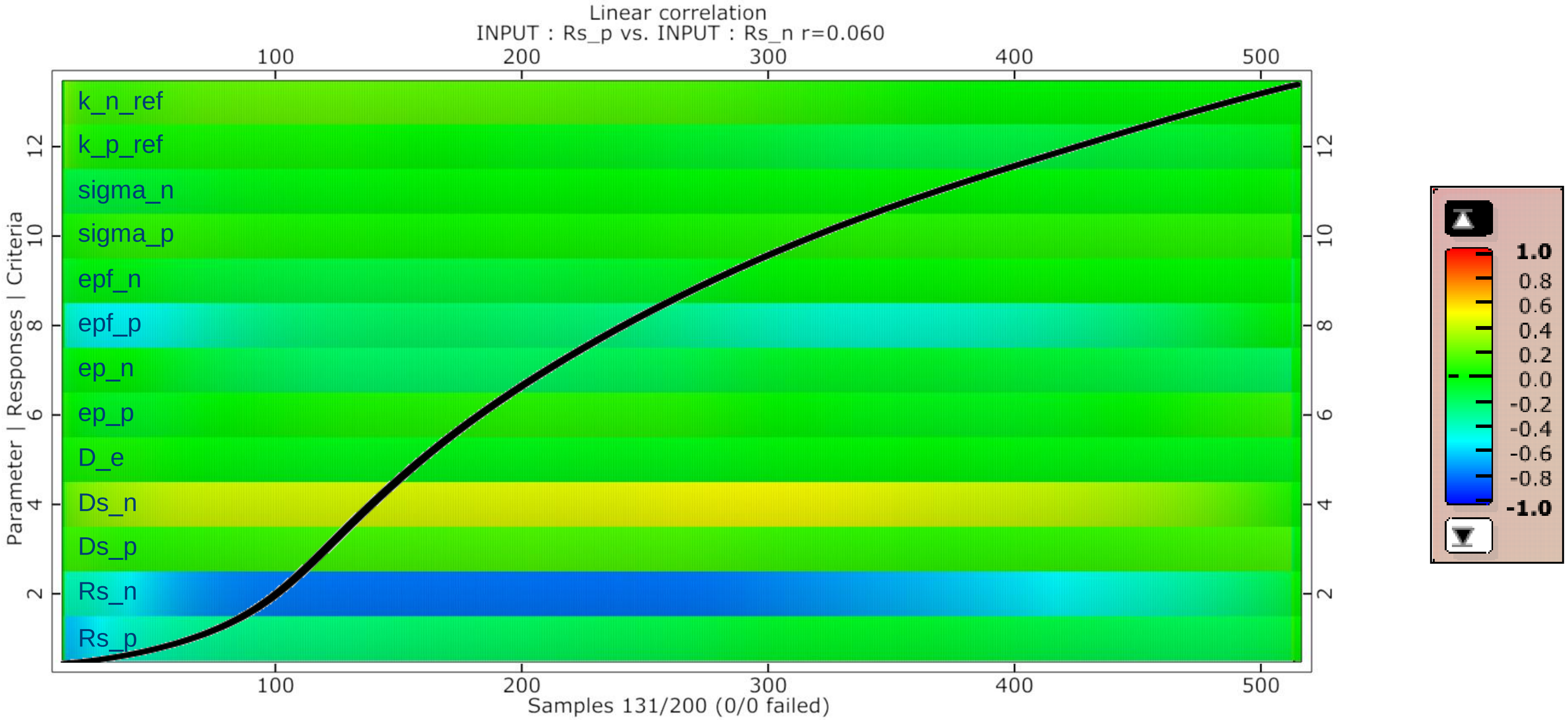
- 1^{st} sensitivity with 200 designs
  - Statistics
    - Unconverged solutions: 34
    - Limit of 2.75 V not reached: additional 128 designs
    - Non-valid designs: 162
    - Valid designs: 38

- 2^{nd} sensitivity with 200 designs
  - Reduction of parameter bounds based on designs with low difference values

  → Identify parameters with high influence on the signal
  - Statistics
    - Unconverged solutions: 0
    - Limit of 2.75 V not reached: additional 69 designs
    - Non-valid designs: 69
    - Valid designs: 131

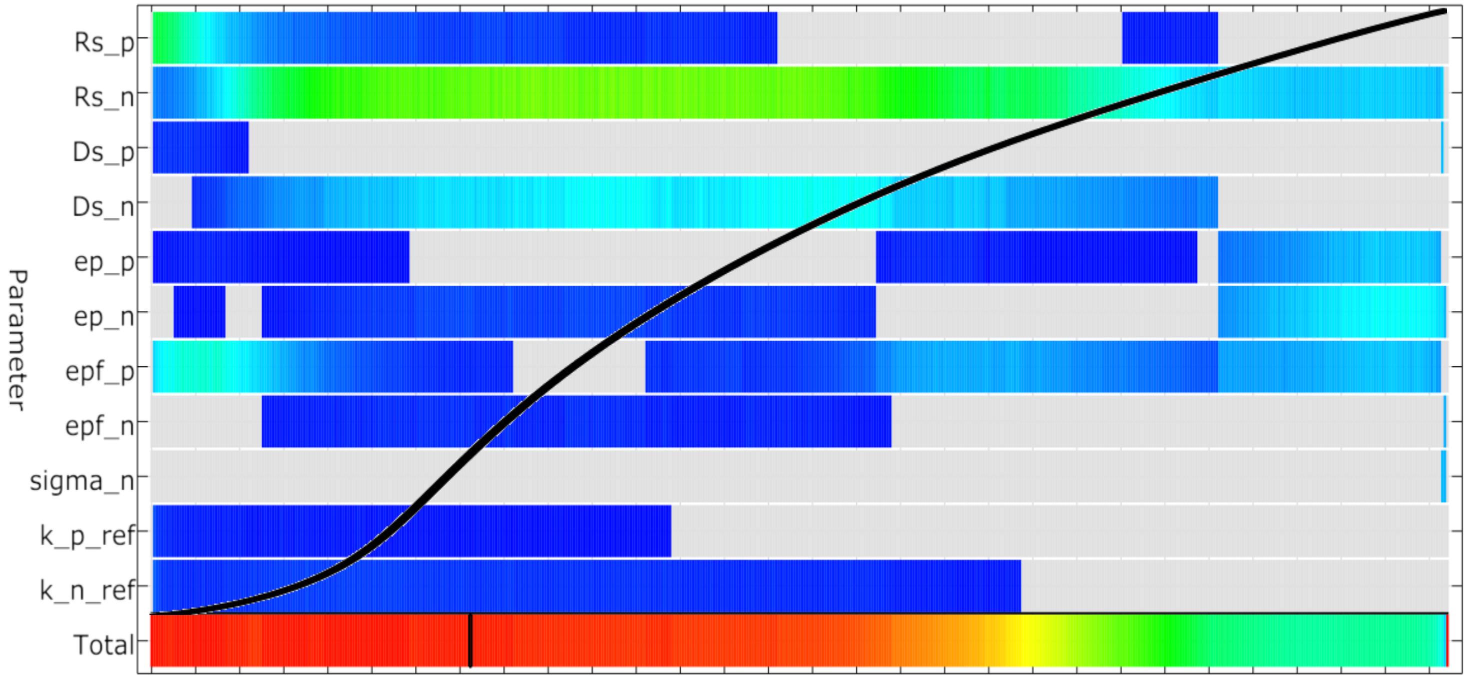
Influence of Input Parameters on Signal

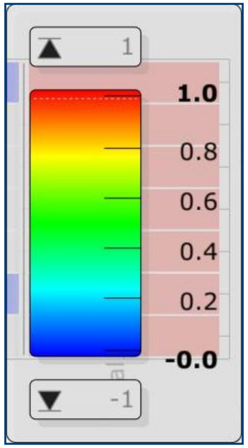
- Linear correlation matrix
  - Resolution of signal with 500 sampling points



Influence of Input Parameters on Signal

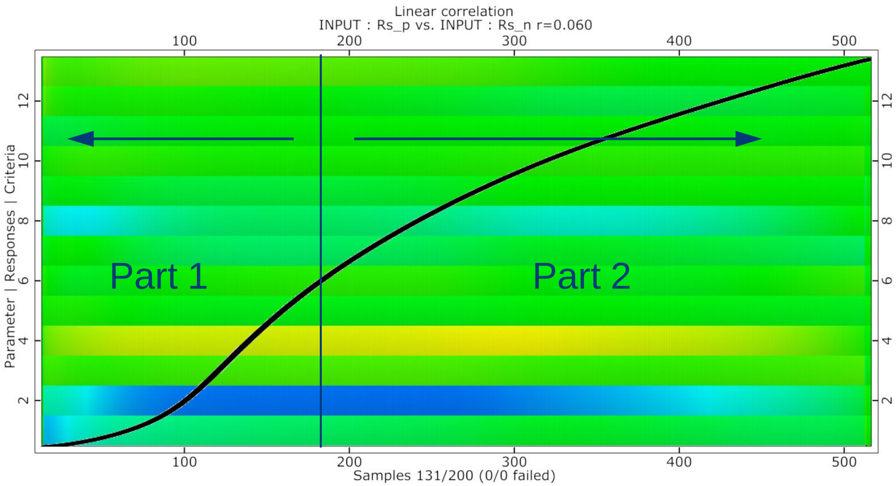
- COP Matrix
  - 11 important parameters
  - 2 unimportant parameters (D_e and sigma_p)





Calibration – Minimize Difference between Reference and Simulation

- Dividing signals in 2 parts
  - Differenced for part 1 and part 2 for all C rates



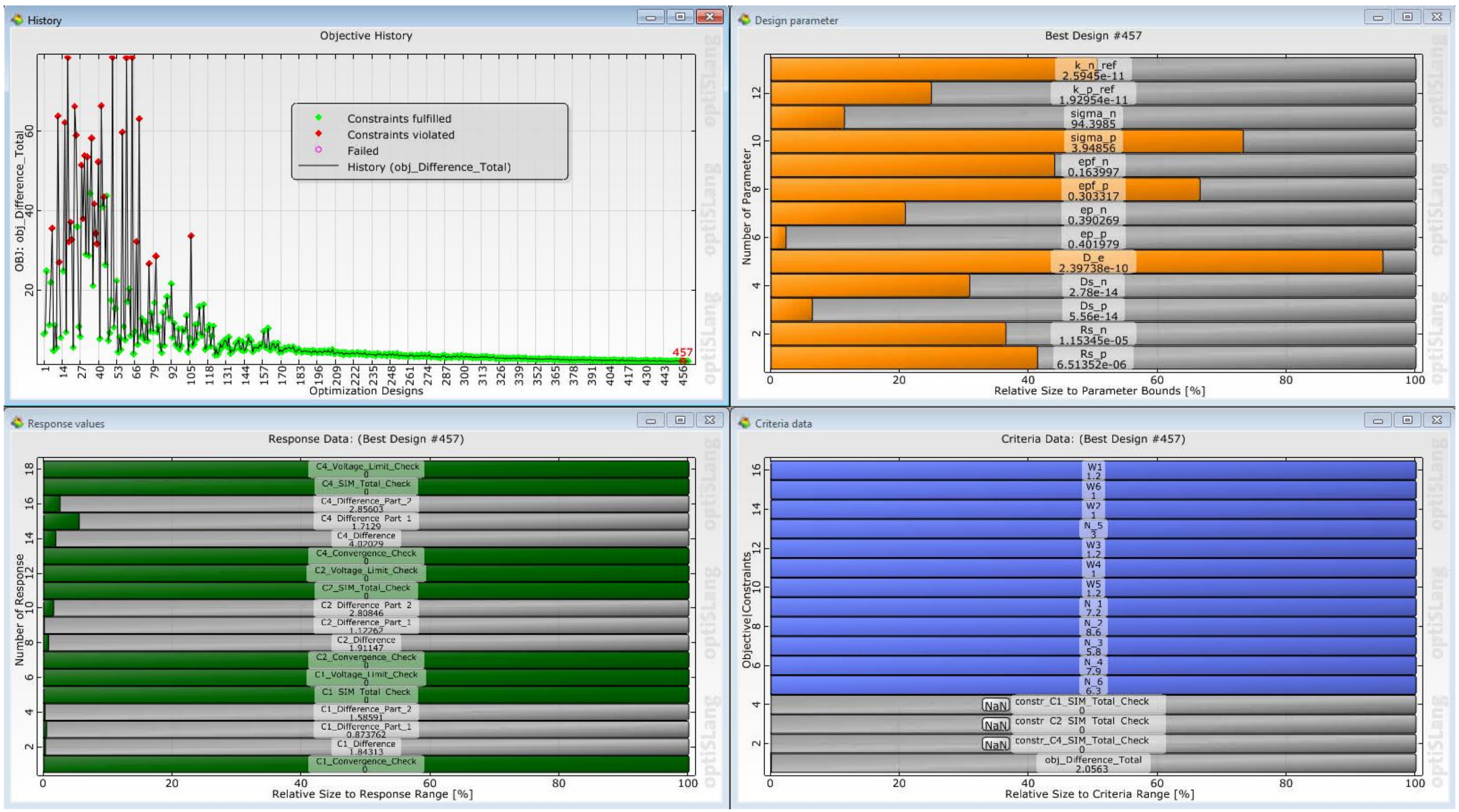
- Restrictions
  - All check output parameters >= 0

- Weighting factors: W_i
- Normalizing factors: N_i (max y-value minus min y-value)

- Objective function
  - **min (W_1*C1_Difference_Part 1/N_1 + W_2*C1_Difference_Part 2/N_2 …)**

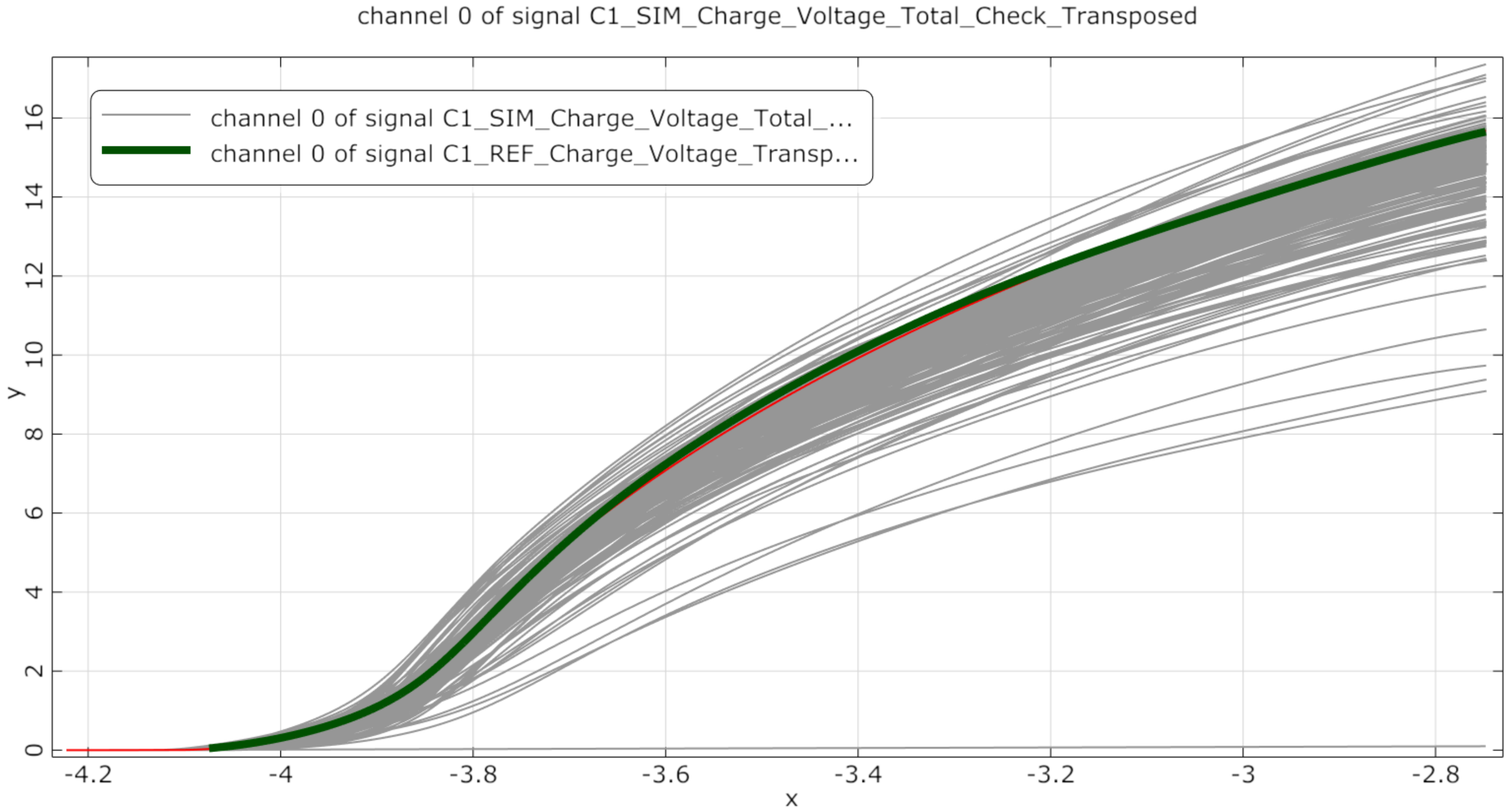
Optimization Results

- Adaptive Response Surface Optimization

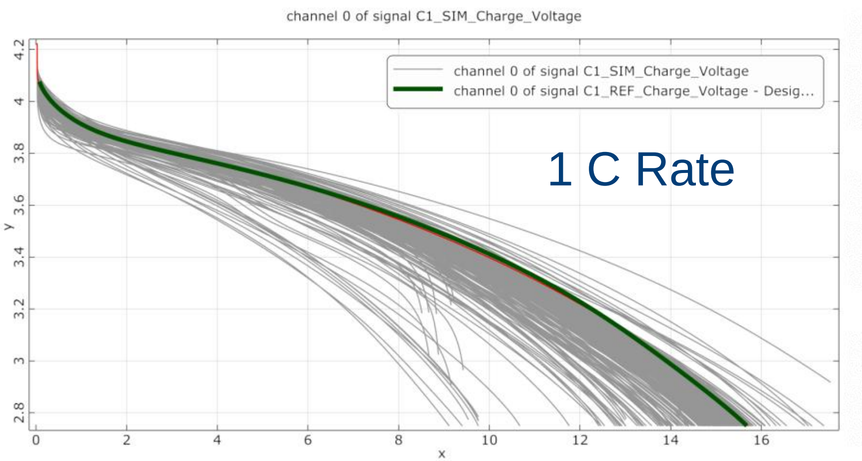


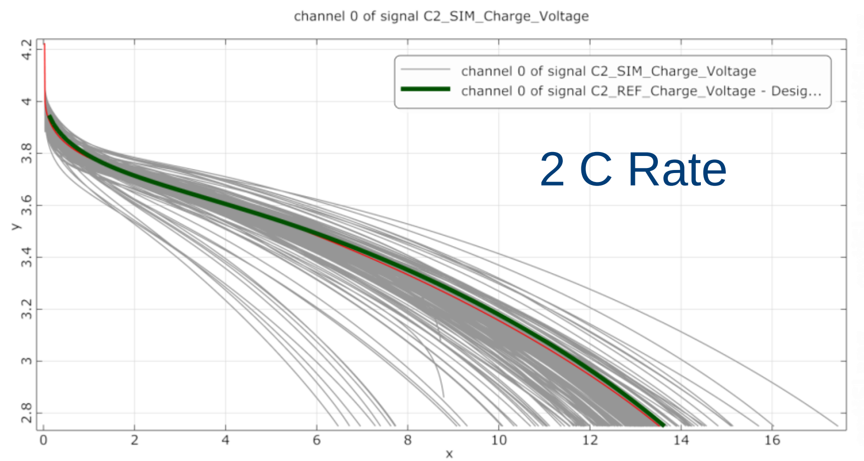
Optimization Results

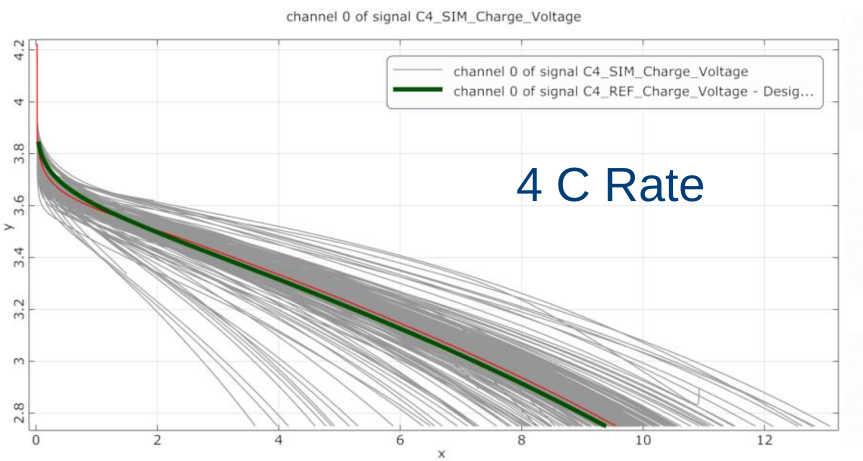
- Transposed 1 C Rate



Optimization Results

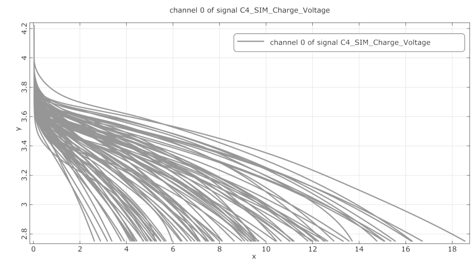






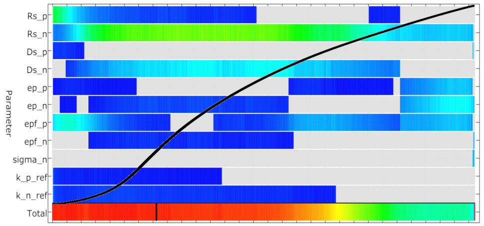
Summary

- Parametric simultaneous simulation of battery discharge behavior for different C rates

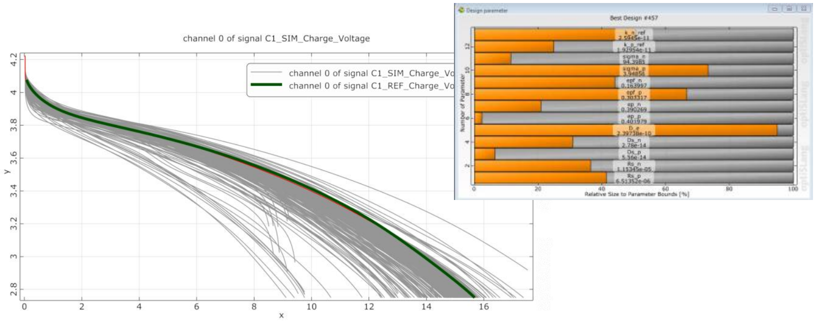


- Signal lengths differ → transposing signals

- Sensitivity reveals parameters influencing the signal characteristic



- Minimizing the difference between reference and simulation by optimization
- Determination of battery parameters



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