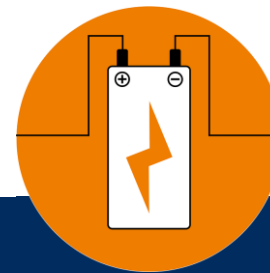




Simulation ist mehr als Software®



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

Nico Nagl – CADFEM GmbH  
Lucas Kostetzer – CADFEM GmbH

## 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

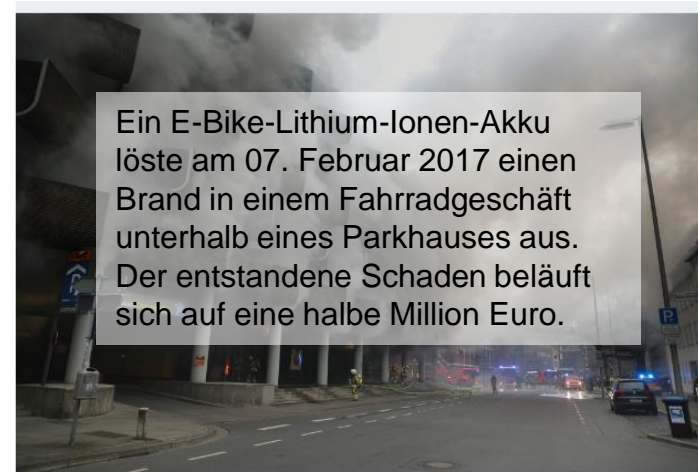
9. Oktober 2016, 18:57 Uhr Brennende Akkus

### Schwelendes Verfahren



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

Quelle: [www.sueddeutsche.de](http://www.sueddeutsche.de)



Ein E-Bike-Lithium-Ionen-Akku löste am 07. Februar 2017 einen Brand in einem Fahrradgeschäft unterhalb eines Parkhauses aus. Der entstandene Schaden beläuft sich auf eine halbe Million Euro.

Quelle: [www.all-electronics.de](http://www.all-electronics.de)

# CADFEM<sup>®</sup>



Simulation ist mehr als Software<sup>®</sup>

## 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:

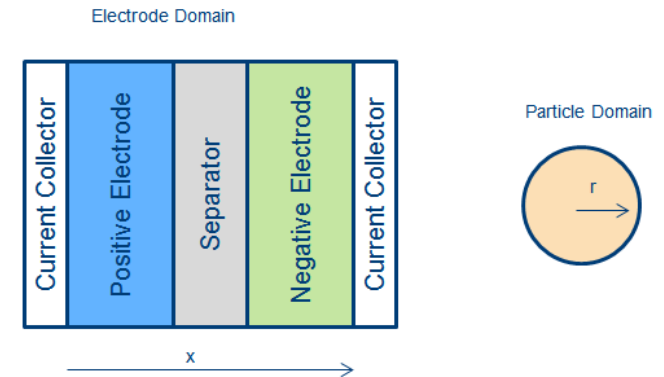
### Dimension x:

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

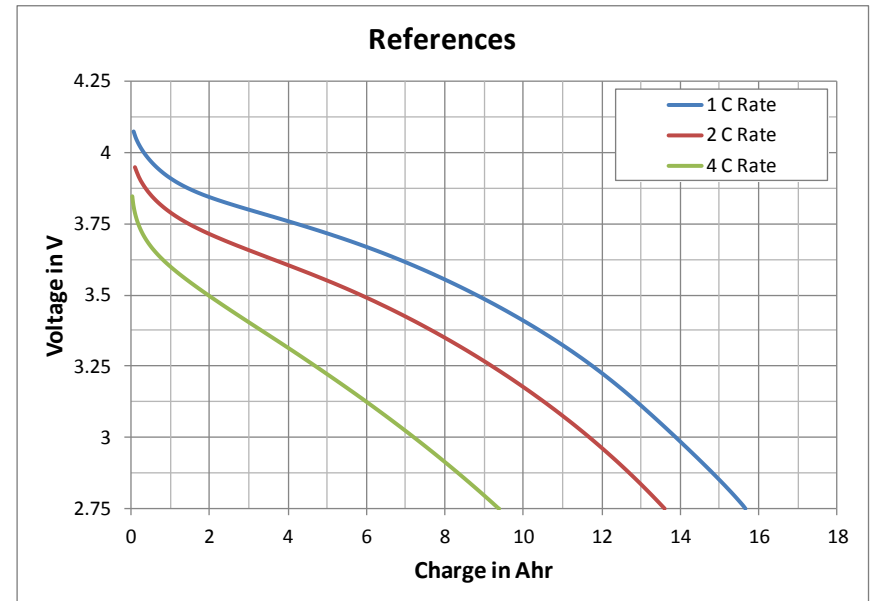
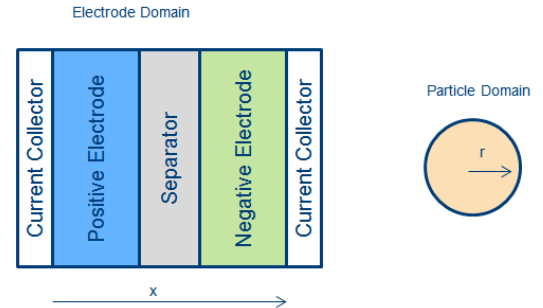


```

C:\Windows\system32\cmd.exe
BF_sun_c (p,n) = -1.155403e-004 , 1.155353e-004
coef. loop= 6
time step = 1.000000e+000
RMS_change_phy_s = 2.641180e-006
RMS_change_phy_e = 1.587784e-006
RMS_change_c = 8.499010e-005
RMS_change_cs = 4.430842e-005
RMS_phy_s = 2.421626e-009
RMS_phy_e = 4.083179e-013
RMS_c = 1.850237e-005
RMS_cs = 1.521184e-027
Imbalance_c = 2.521560e-010
Imbalance_I = 4.784801e-003
Imbalance_cs = 3.130614e-009
Imbalance_cs_loc = 25
BF_sun_curr (p,n) = -17.50 , 17.50
BF_sun_c (p,n) = -1.155382e-004 , 1.155355e-004
time step converged
Voltage limit reached
iteration = 16893
time = 3.065000e+003
Drücken Sie eine beliebige Taste . . .
    
```

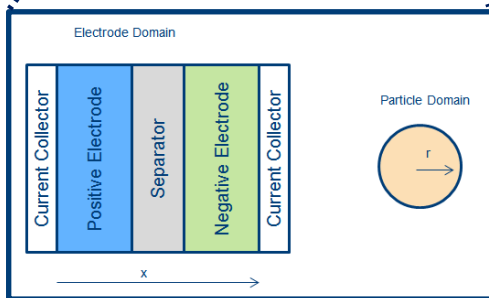
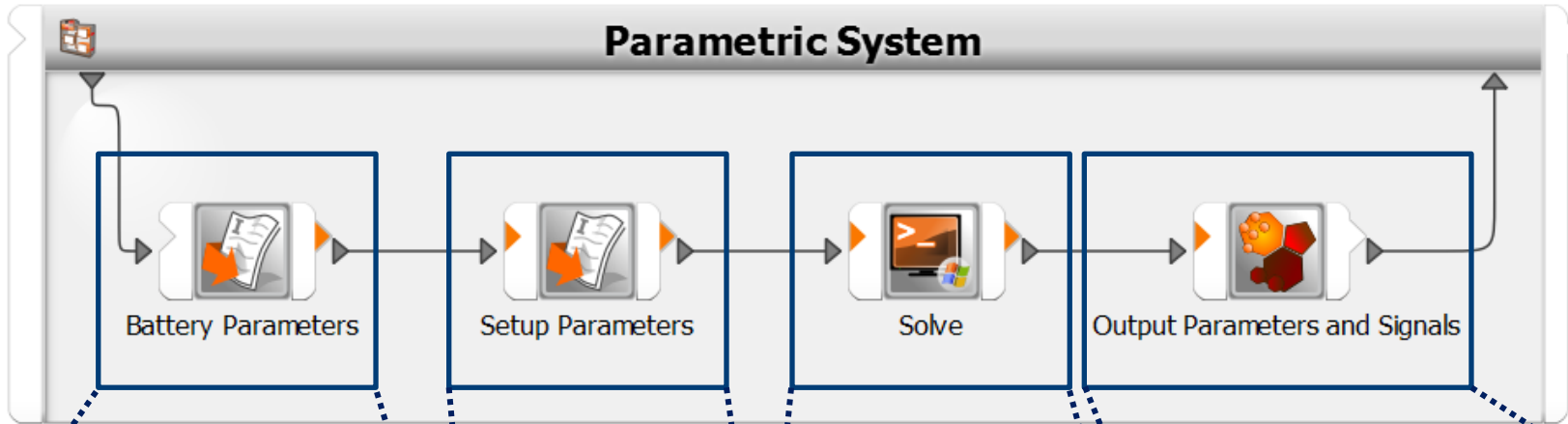
# Parametric Workflow for Battery Simulation

- 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

### Parametric System



```

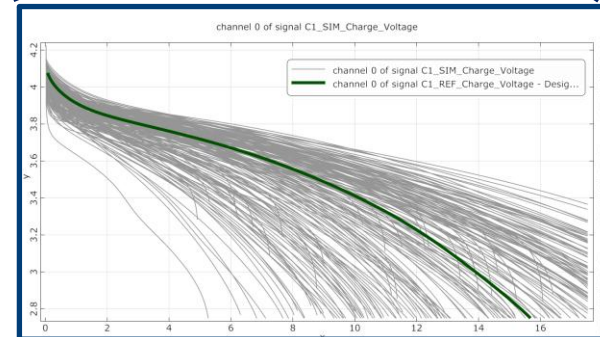
1 current_pos 17.500000000000000
2 T 298.000000000000000
3 v_min 3.000000000000000
4 v_max 4.500000000000000
5 N_p 10.000000000000000
6 N_s 10.000000000000000
7 N_n 10.000000000000000
8 N_par 15.000000000000000
9 dt 1.000000000000000
10 dtmin 1.000000000000000
11 dtmax 1.000000000000000
12 finalt 3320.0000000000000
13 ncl 100.000000000000000
14 sub_it_max_phy_s 5.000000000000000
15 relax_phy_s 1.000000000000000
16 relax_phy_e 1.000000000000000
17 RMS_criteria 0.000100000000000
18 imbalance_criteria 0.010000000000000
19 console_output_level 1.000000000000000
20

```

```

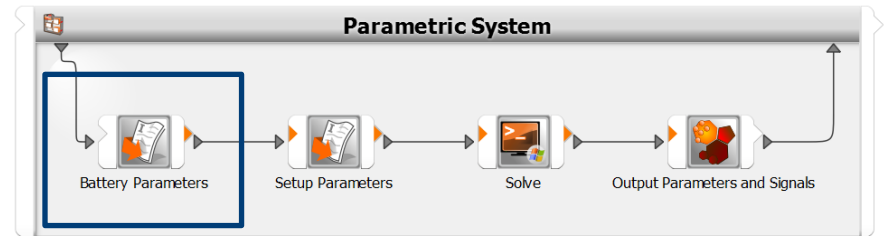
C:\Windows\system32\cmd.exe
BF_sun_c <p,n> = -1.155403e-004 , 1.155353e-004
coef_loop= 6
Cline stop
RMS_change_phy_s = 1.000000e+000
RMS_change_phy_e = 2.641180e-006
RMS_change_cs = 1.587784e-006
RMS_change_sc = 8.492818e-005
RMS_change_scs = 4.438842e-005
RMS_phy_s = 2.421626e-009
RMS_phy_e = 4.883179e-013
RMS_c = 1.858237e-005
RMS_cs = 1.521184e-027
Imbalance_c = 2.521565e-016
Imbalance_l = 4.784801e-003
Imbalance_cs = 3.138614e-009
Imbalance_sc_loc = 25
BF_sun_cupr <p,n> = -17.50 , 17.50
BF_sun_c <p,n> = -1.155382e-004 , 1.155355e-004
time step converged
Voltage limit reached
iteration = 16893
Cline = 3.865088e+089
Drücken Sie eine beliebige Taste . . .

```



# Battery Parameters and Ranges for Sensitivity Analysis

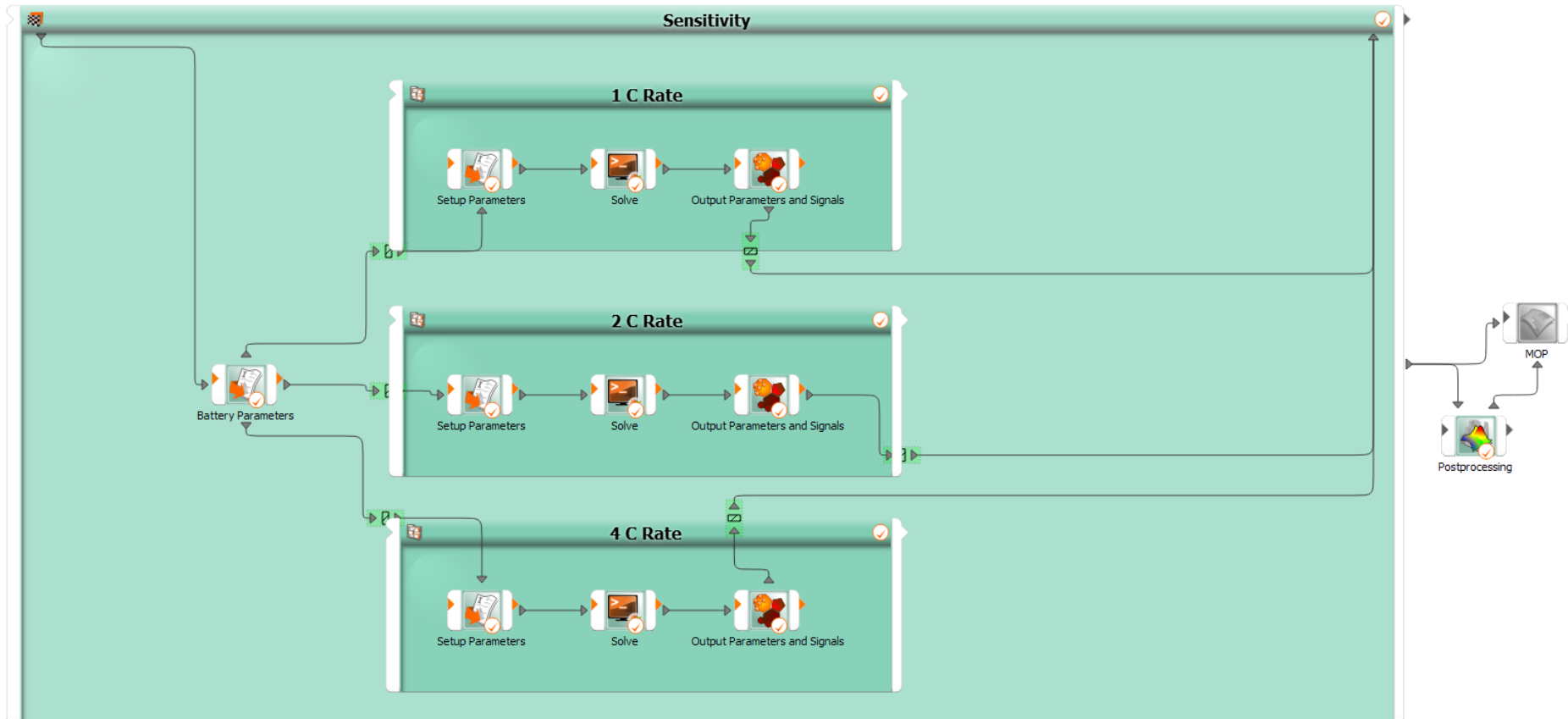
- 13 Input Parameter
  - Which parameters influence the discharge signal?
- Sensitivity analysis



Name	Description	Unit	Reference Value	Lower Bound	Upper Bound
D_e	electrolyte phase Li-ion diffusion coefficient	m <sup>2</sup> /s	7.50E-11	3.00E-11	1.20E-10
Ds_n	diffusion coefficient at the solid phase. negative electrode	m <sup>2</sup> /s	3.90E-14	1.56E-14	6.24E-14
Ds_p	diffusion coefficient at the solid phase. positive electrode	m <sup>2</sup> /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 <sup>2</sup> /s/(mol/m <sup>3</sup> ) <sup>1.5</sup>	2.33E-11	9.32E-12	3.37E-11
k_p_ref	electrochemical reaction rate constant of positive electrode	mol/m <sup>2</sup> /s/(mol/m <sup>3</sup> ) <sup>1.5</sup>	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

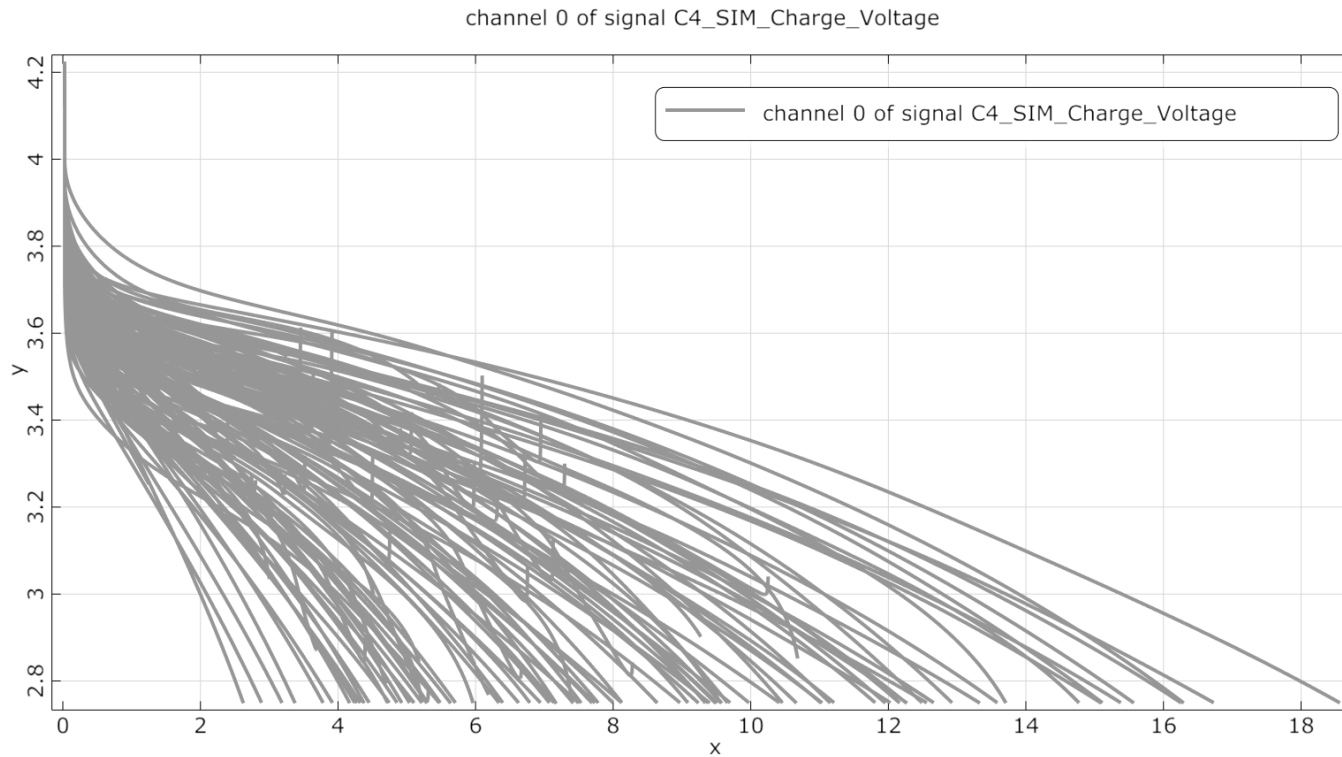
# Simultaneous Simulation Workflow for all 3 C-Rates

- Sensitivity analysis with 200 designs

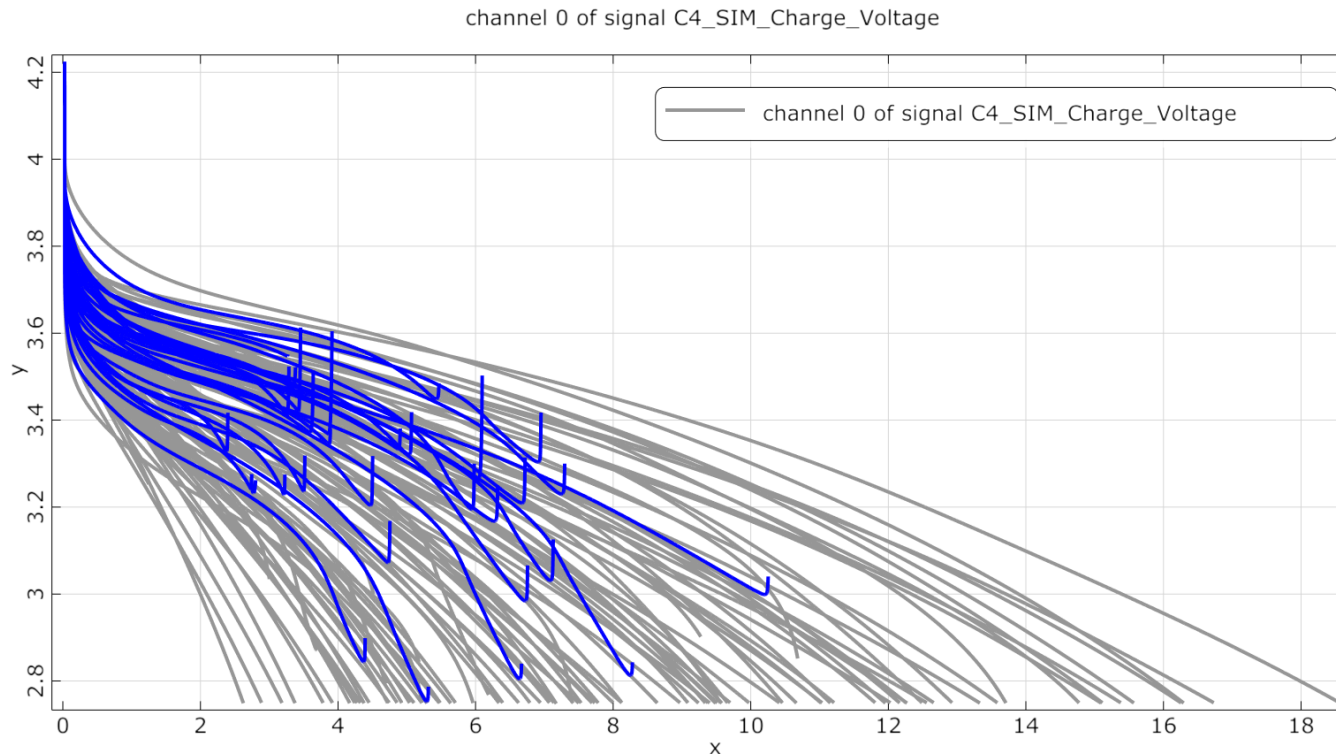




# Characterization of Calculated Signals

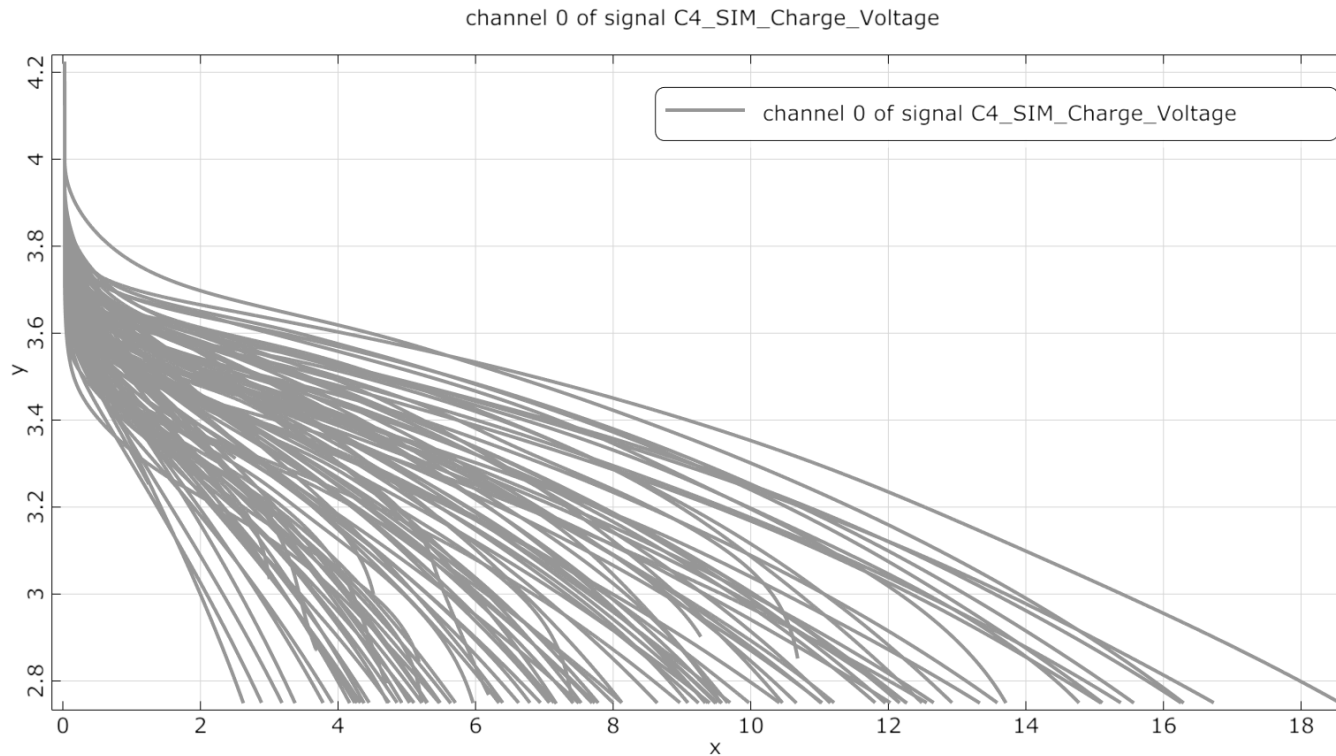


# Characterization of Calculated Signals



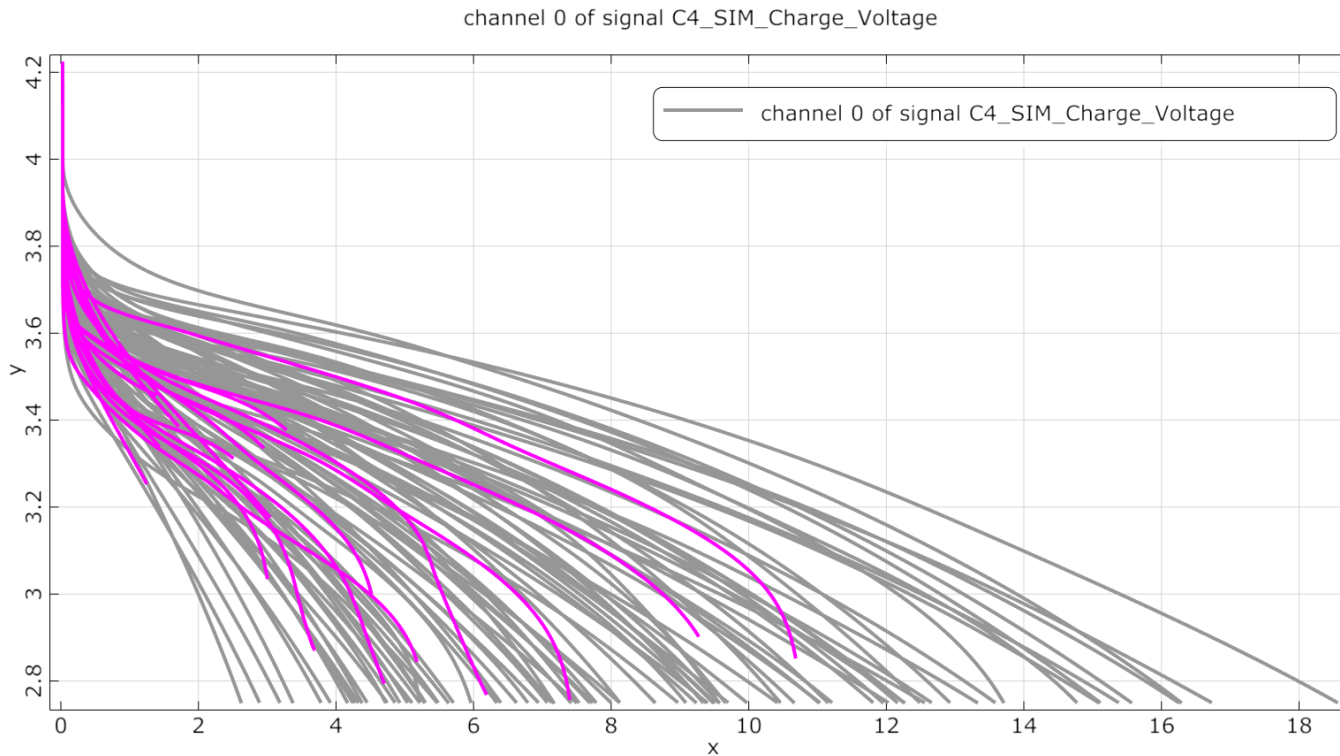
- Non-physical convergence problems → unconverged solution
- New check output parameter: if converged then 0 otherwise -1

# Characterization of Calculated Signals



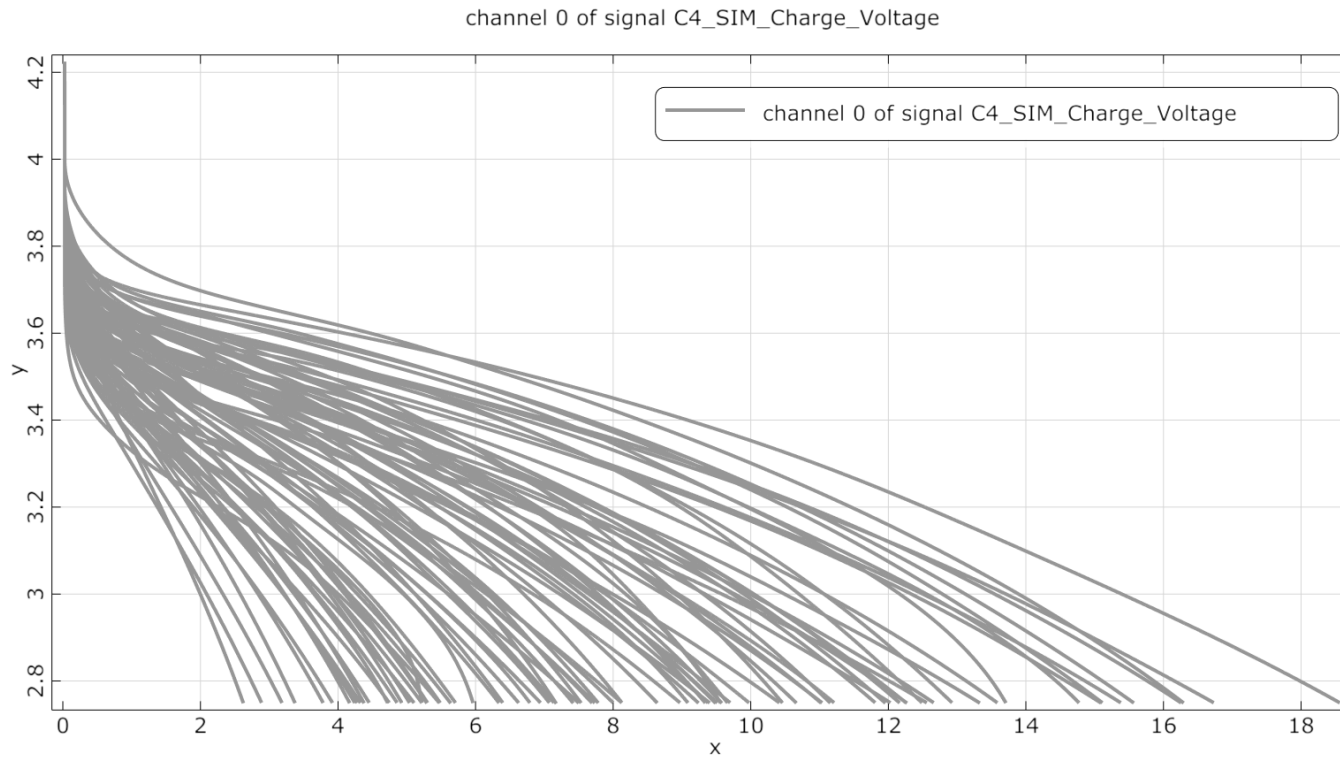
- Unconverged Signals are neglected

# Characterization of Calculated Signals



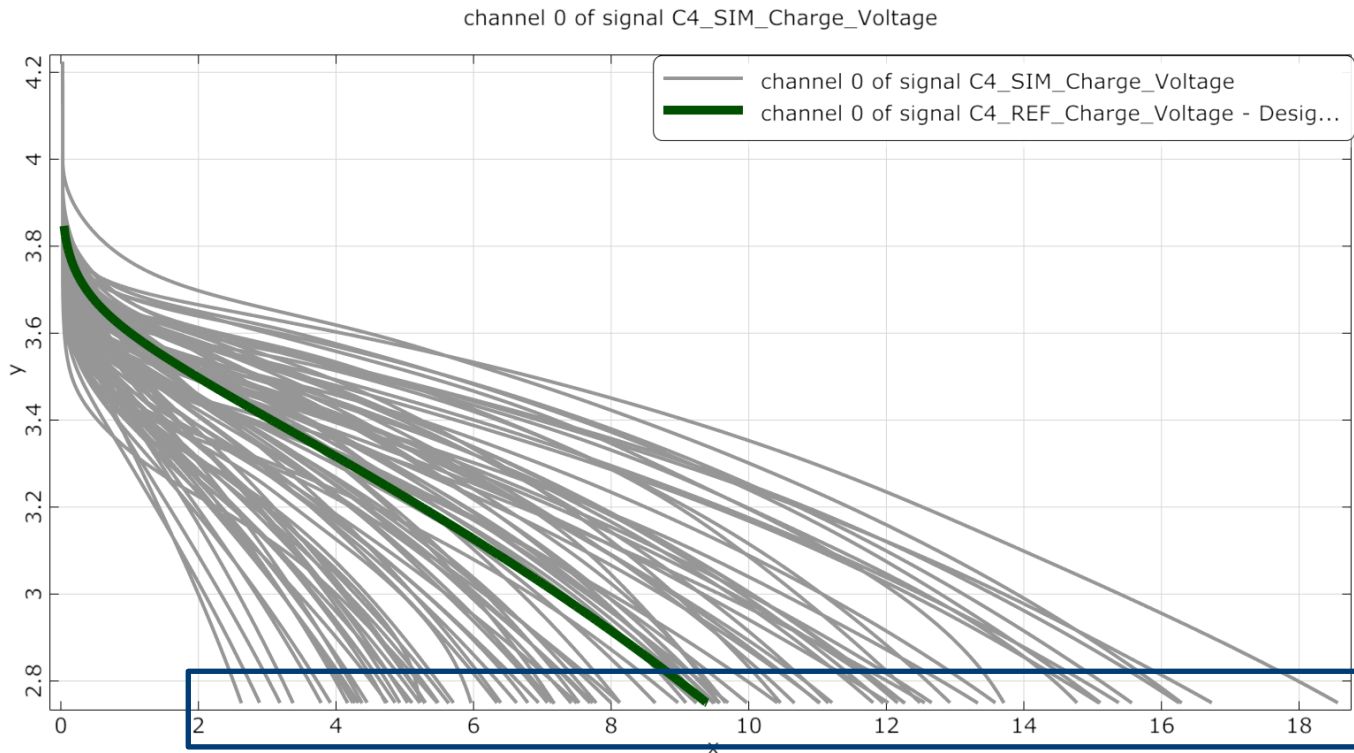
- Limit of 2.75 V is not reached
- Additional check output parameter: if limit reached then 0 otherwise -1

## Characterization of Calculated Signals



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

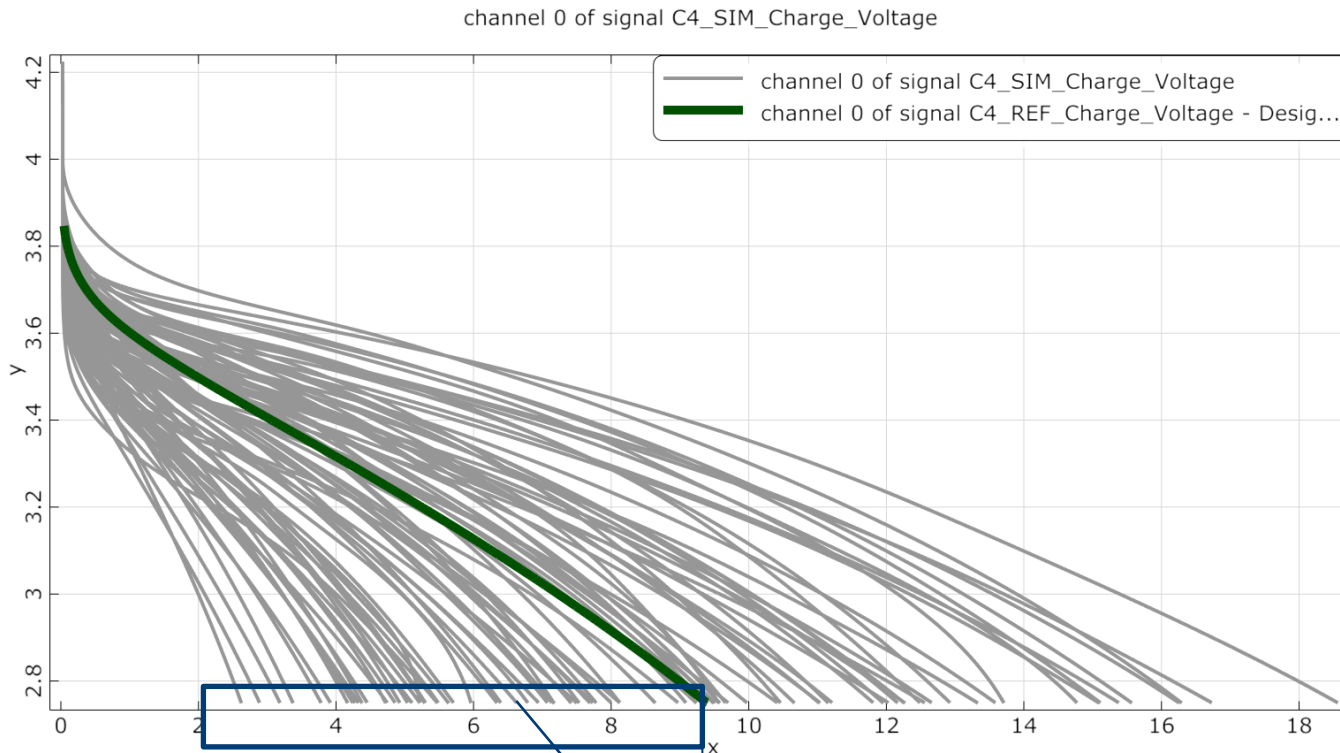
# Characterization of Calculated Signals



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

**BUT**  
**Signal lengths differ!**

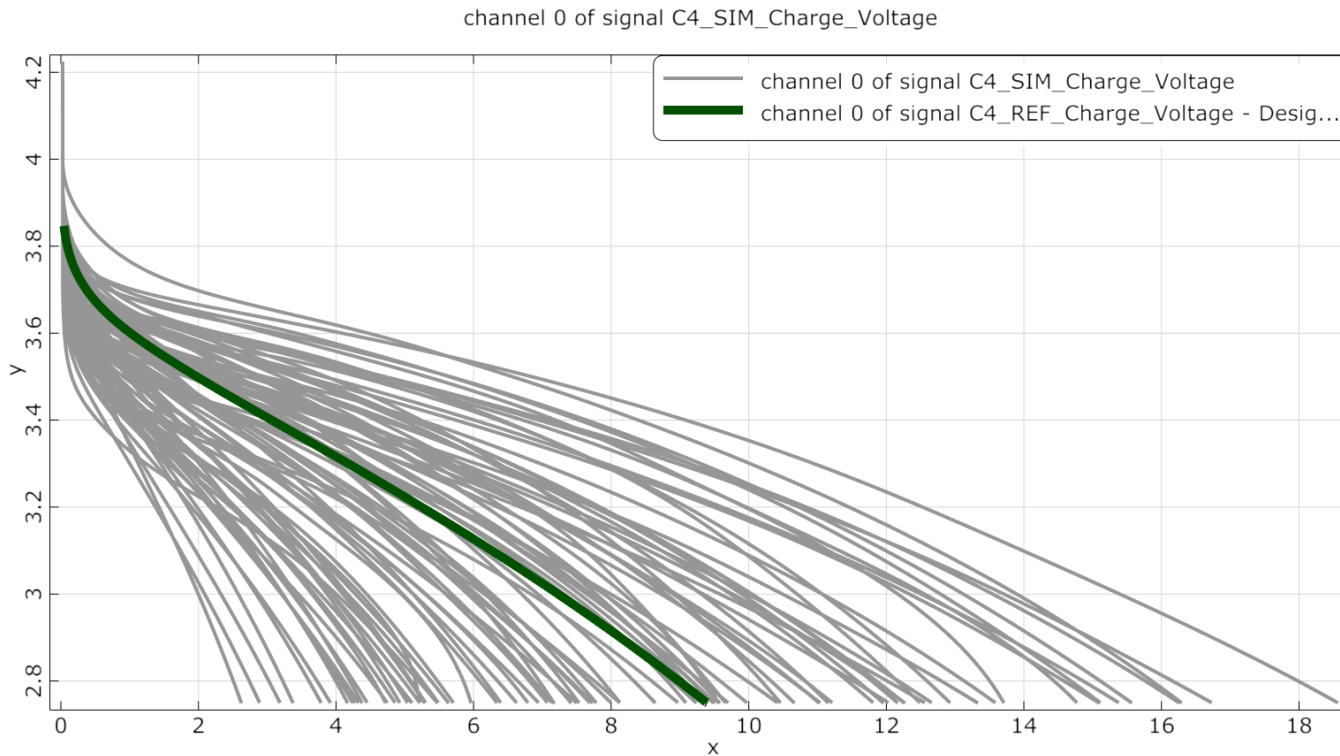
# Characterization of Calculated Signals



- All remaining signals
  - converged
  - reached 2.75 V

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

# Characterization of Calculated Signals



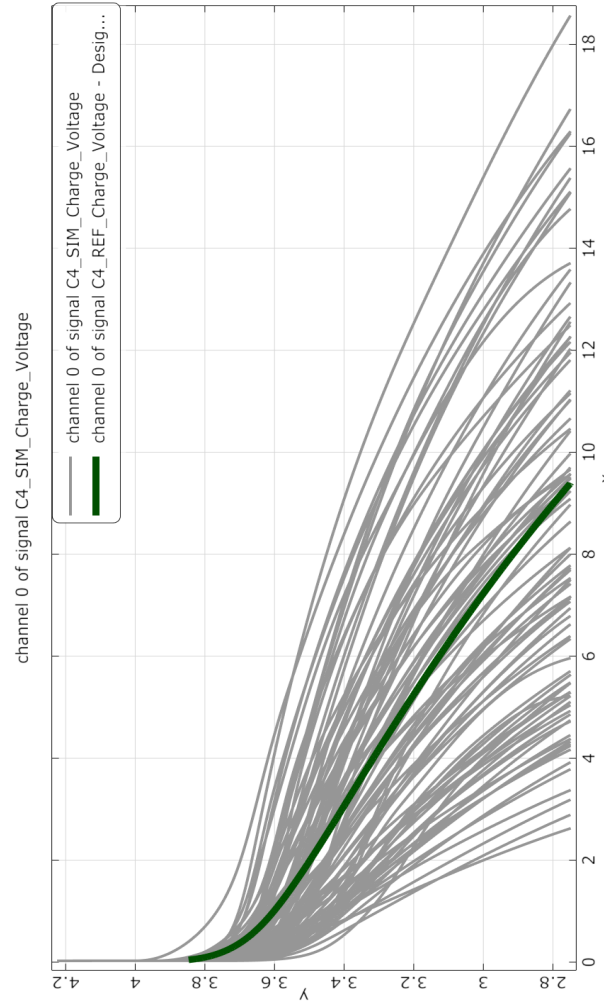
- All remaining signals
  - converged
  - reached 2.75 V

Extrapolation is  
**NO option!**



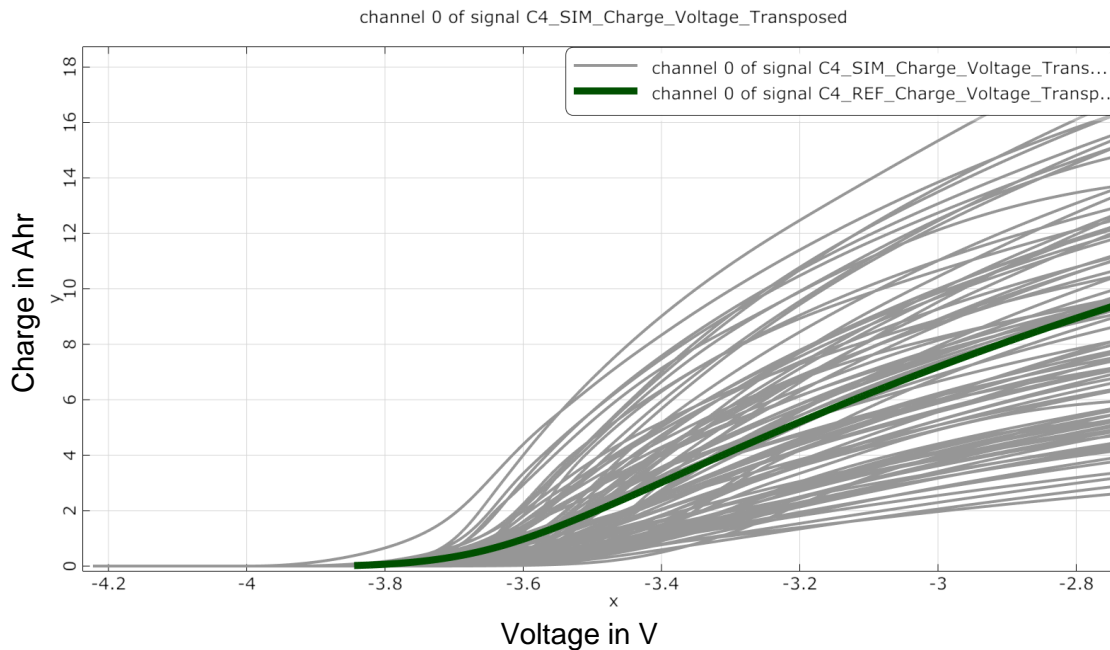
There is a solution  
for this problem!

# Characterization of Calculated Signals



# Characterization of Calculated Signals

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

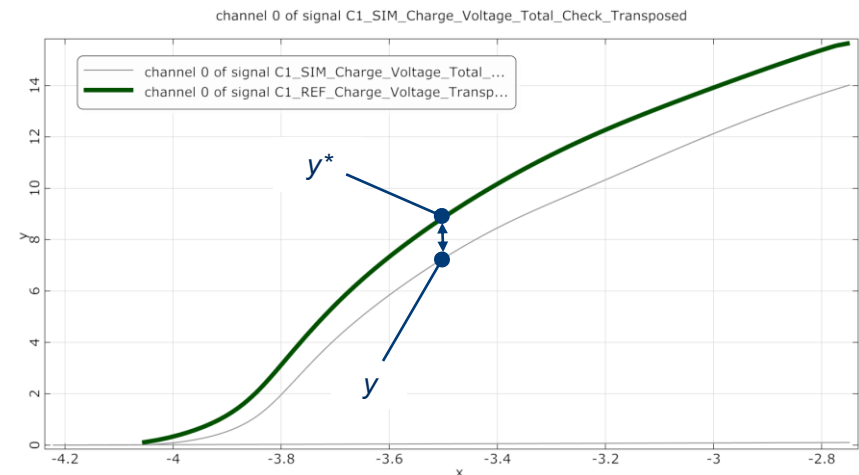


# Calibration – Minimize Difference between Reference and Simulation

- Root Mean Squared Error RMSE (normalized)  $\triangleq$  Difference

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

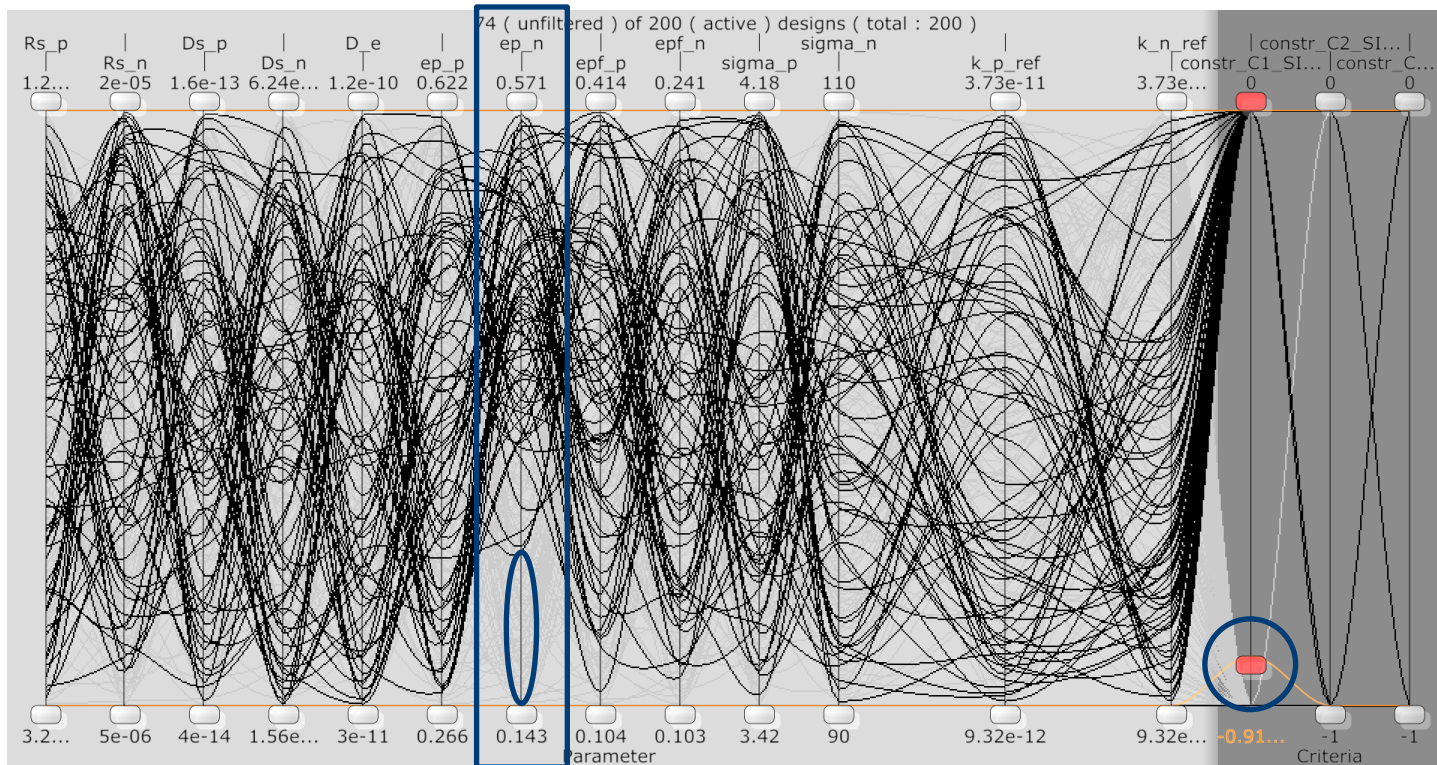
- $n$ : Number of data points
- $y^*$ : Reference value (measurement)
- $y$ : Calculated value (battery simulation)



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

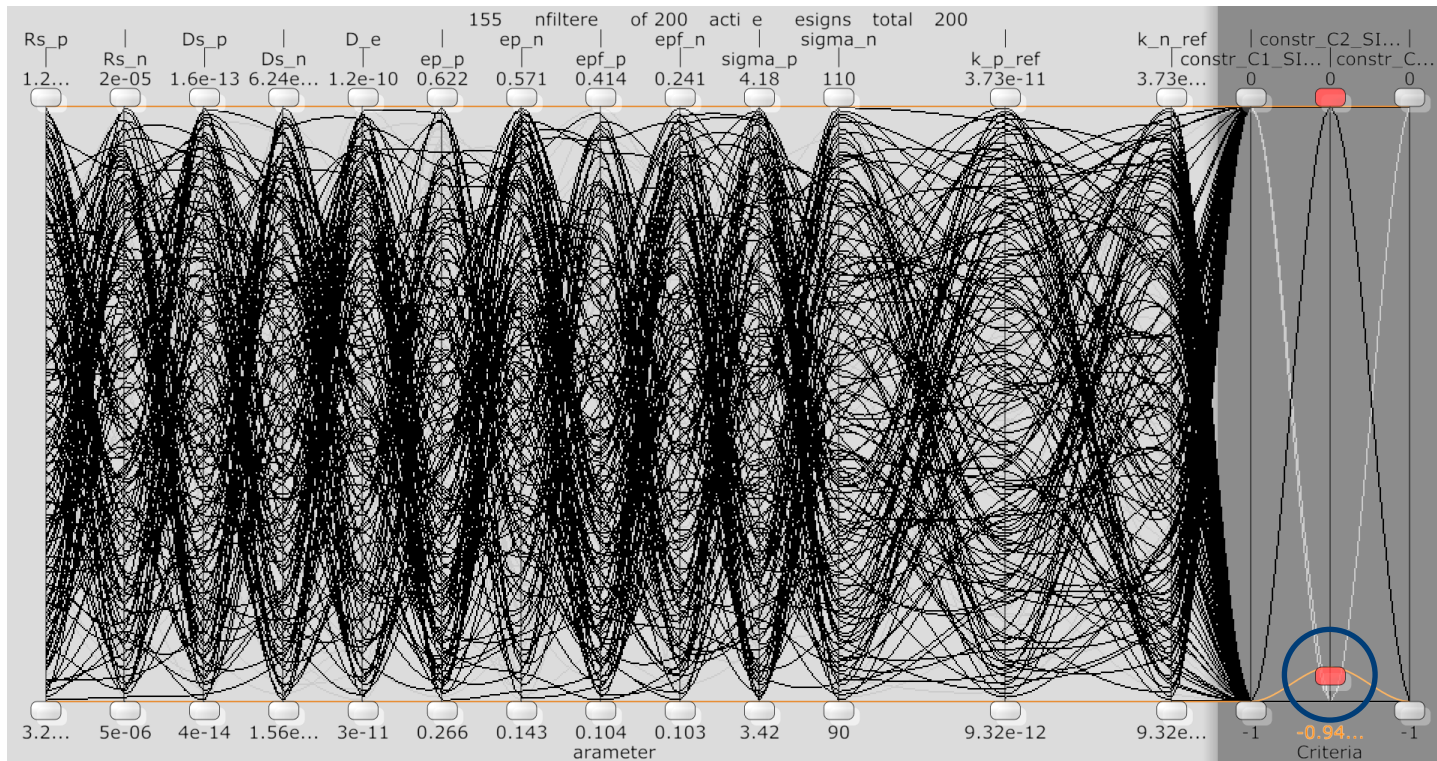
# Identification of non-valid Designs

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



# Identification of non-valid Designs

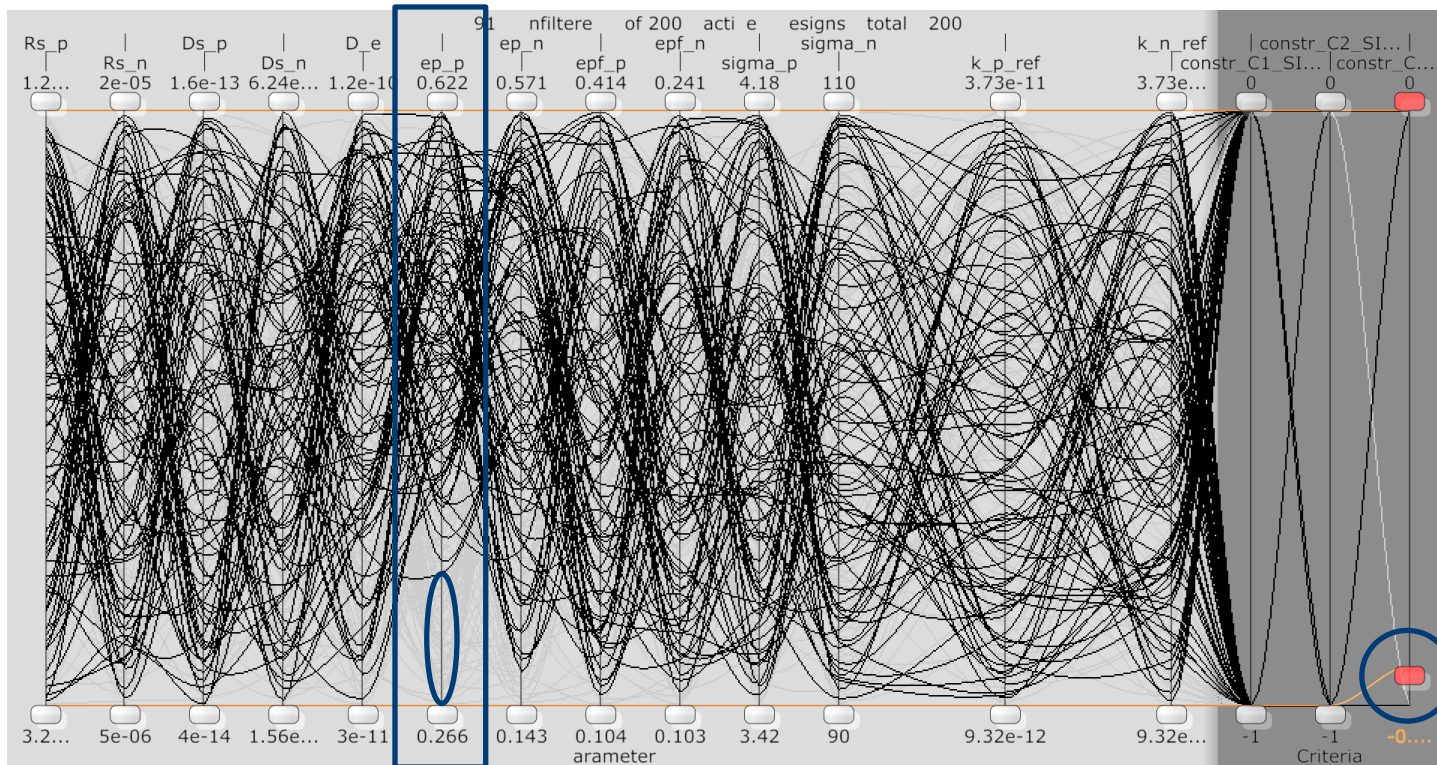
- Parallel Coordinates Plot
  - Designs for check output parameter 2 C rate = -1 are deselected





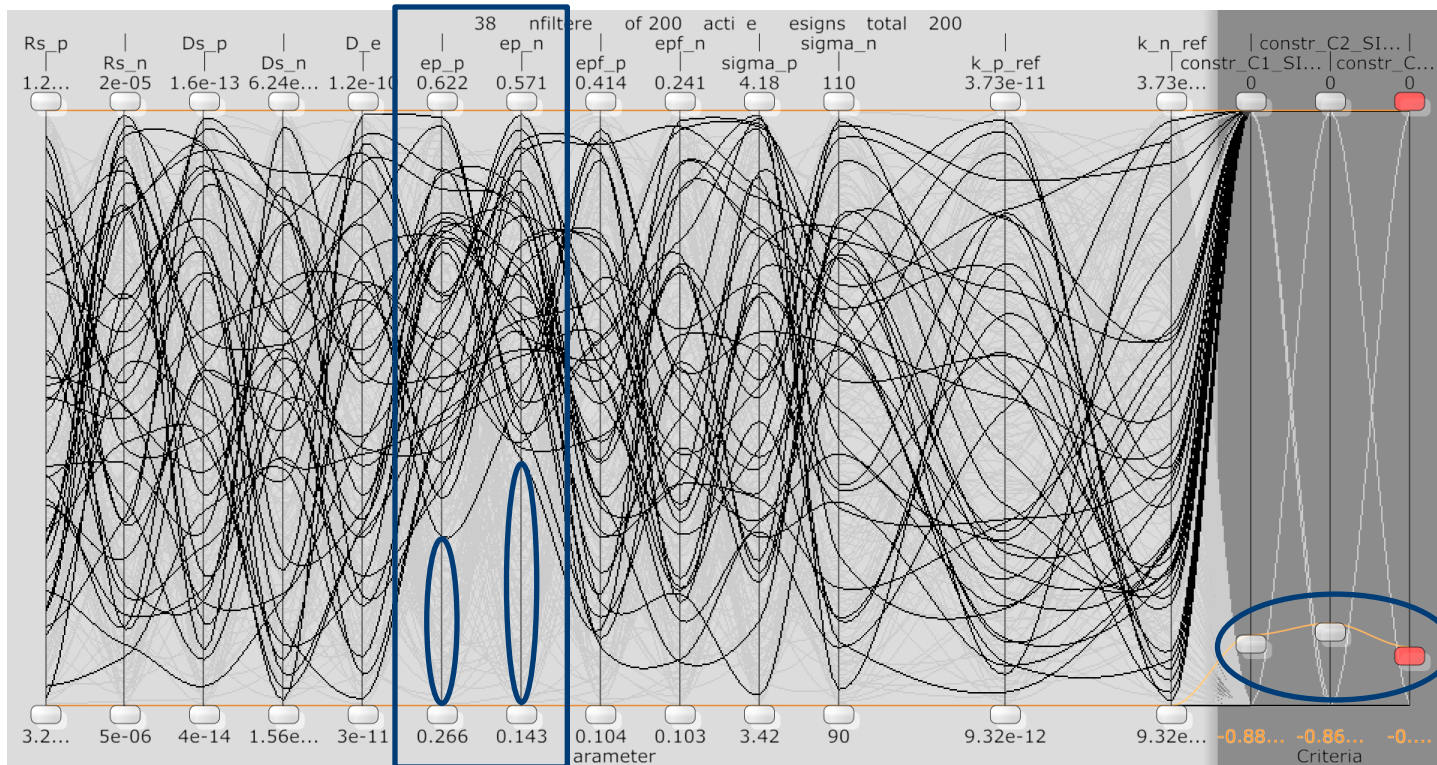
# Identification of non-valid Designs

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



# Identification of non-valid Designs

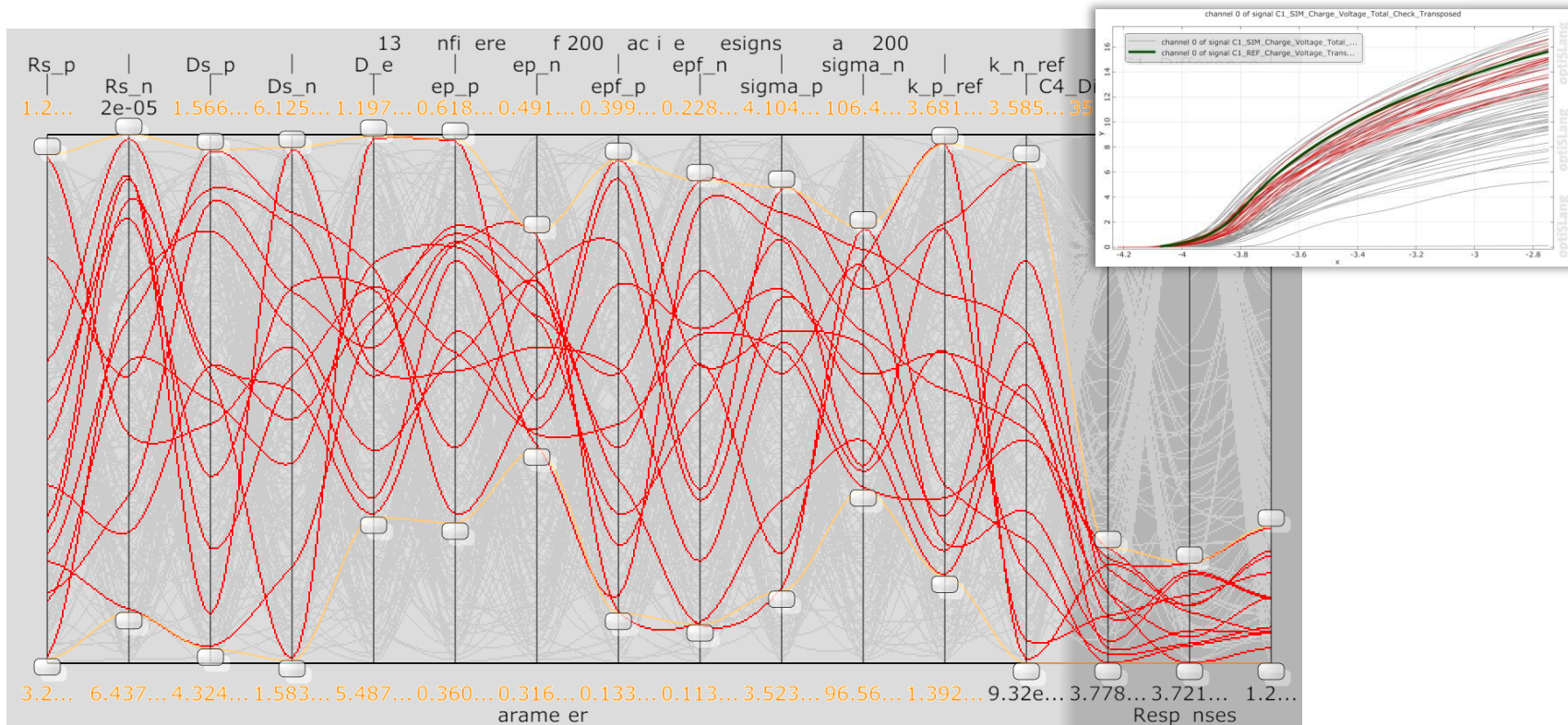
- Parallel Coordinates Plot
  - Designs for check output parameter for all C rates = -1 are deselected





# Identification of non-valid Designs

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

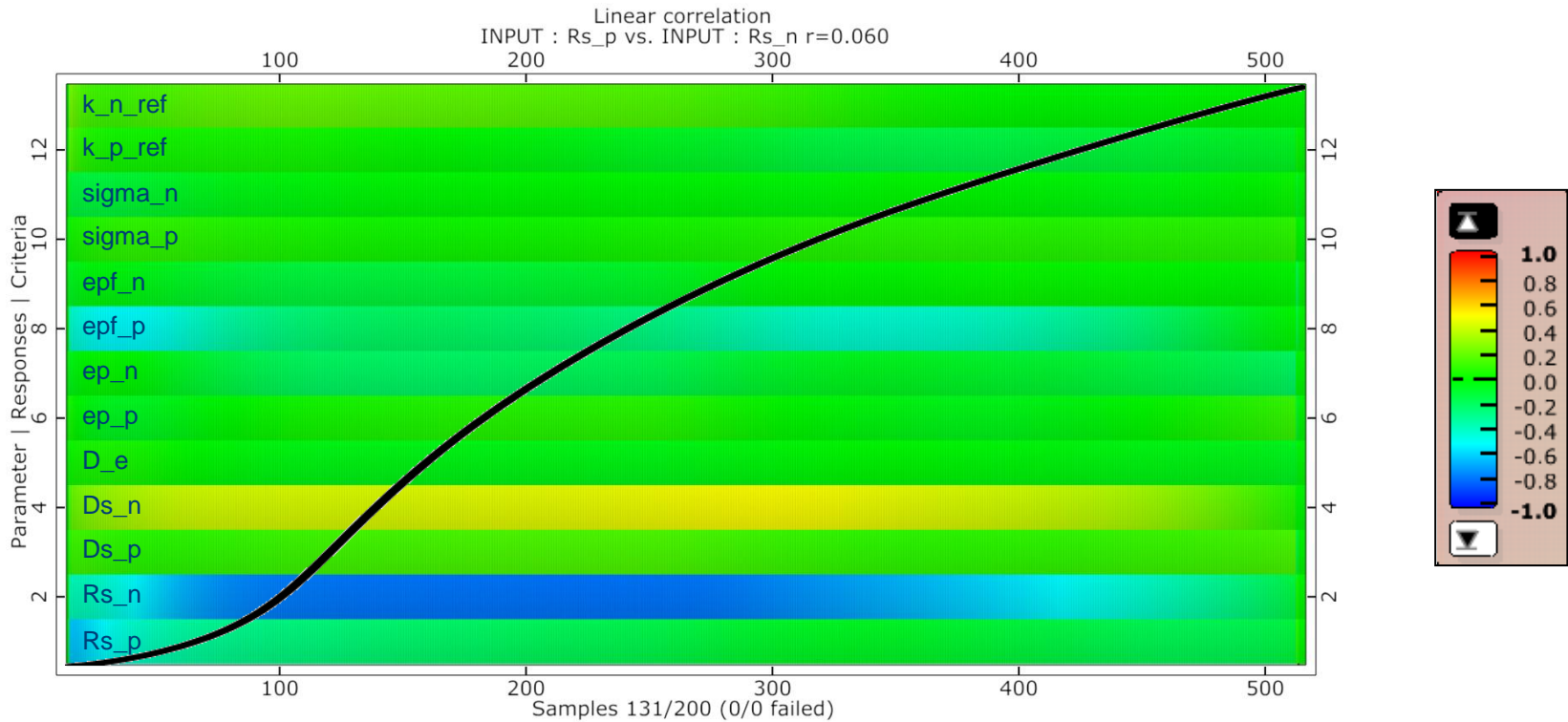


## 2<sup>nd</sup> Sensitivity with Reduced Parameter Bounds

- 1<sup>st</sup> 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<sup>nd</sup> 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

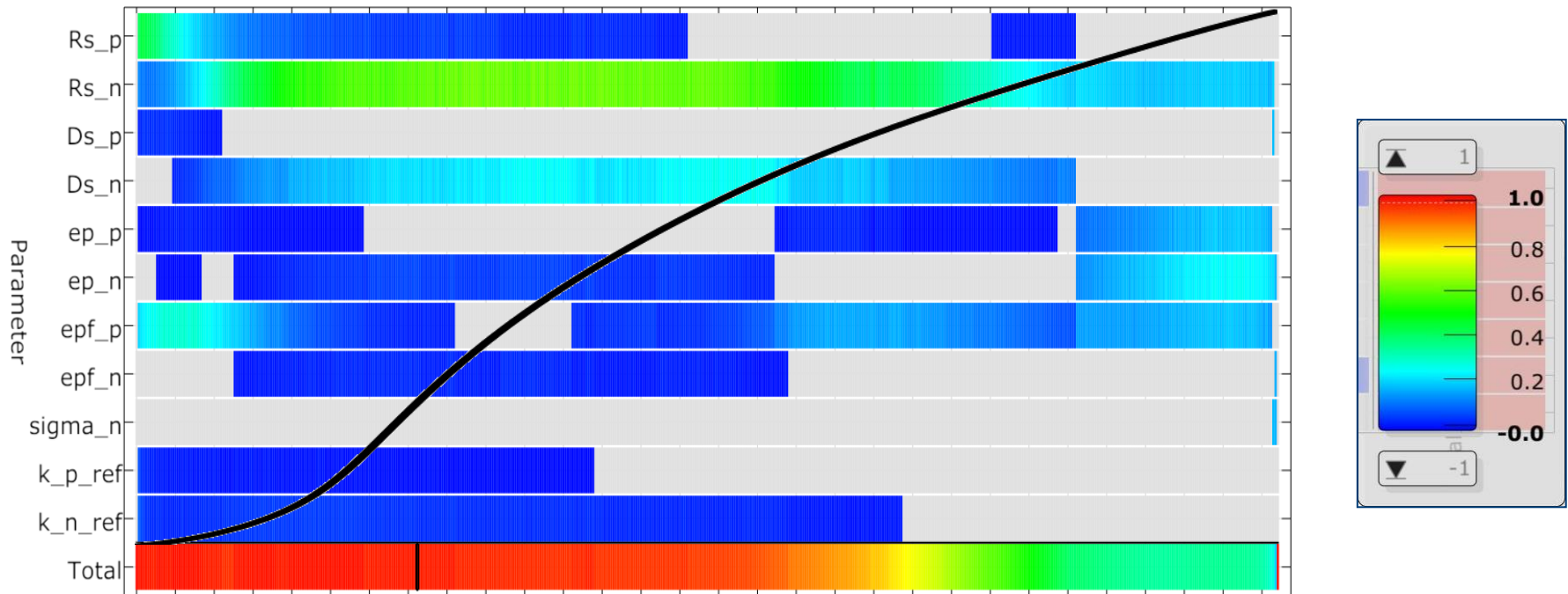
# Influence of Input Parameters on Signal

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



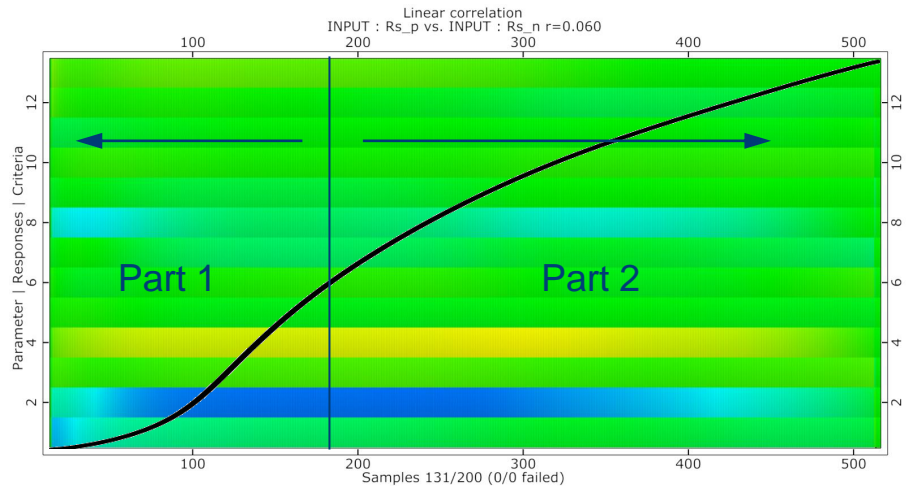
## Influence of Input Parameters on Signal

- 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  $\geq 0$

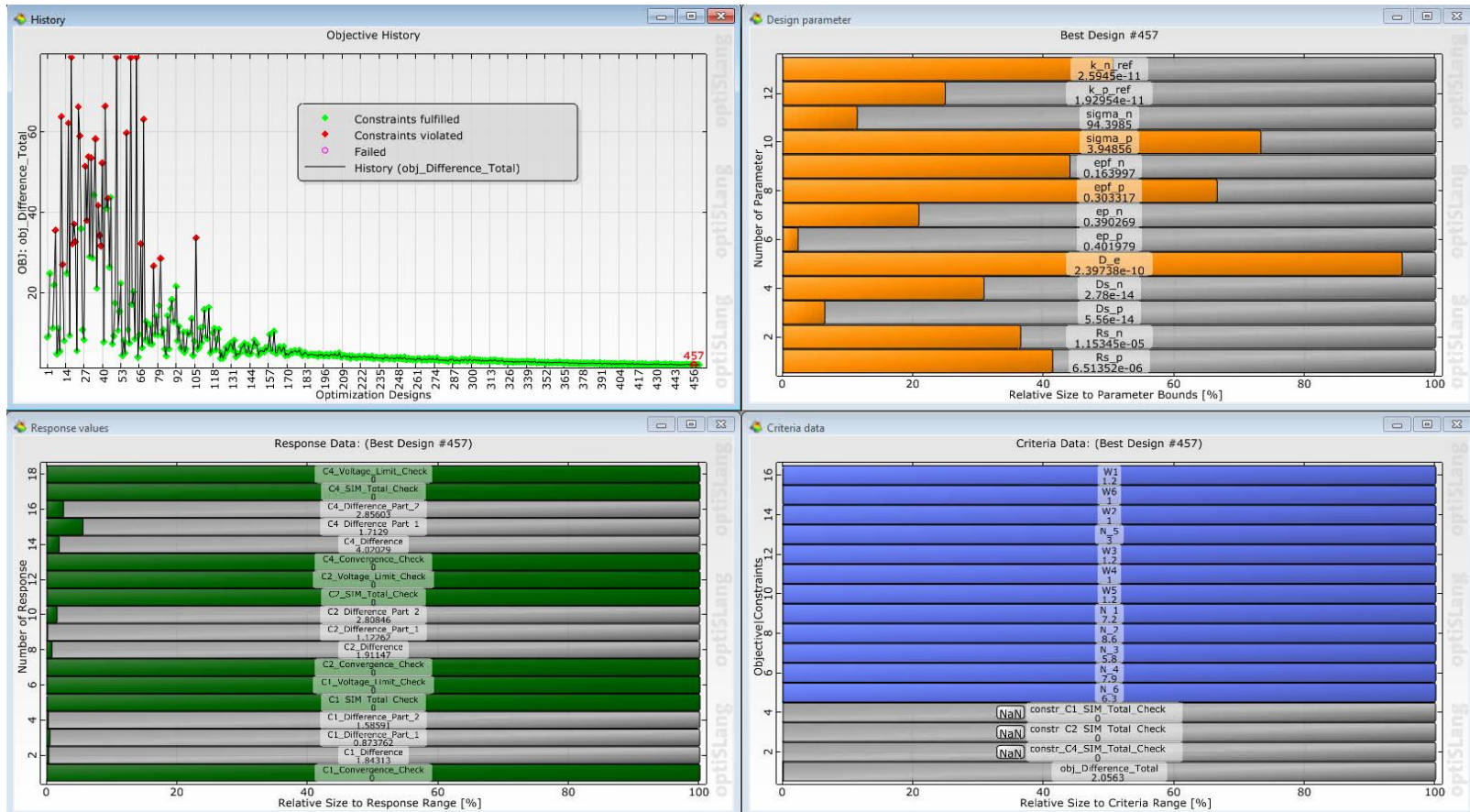


- Weighting factors:  $W_i$
- Normalizing factors:  $N_i$  (max y-value minus min y-value)

- Objective function
  - $\min (W_1 * C1\_Difference\_Part\ 1 / N_1 + W_2 * C1\_Difference\_Part\ 2 / N_2 \dots)$

## Optimization Results

- Adaptive Response Surface Optimization

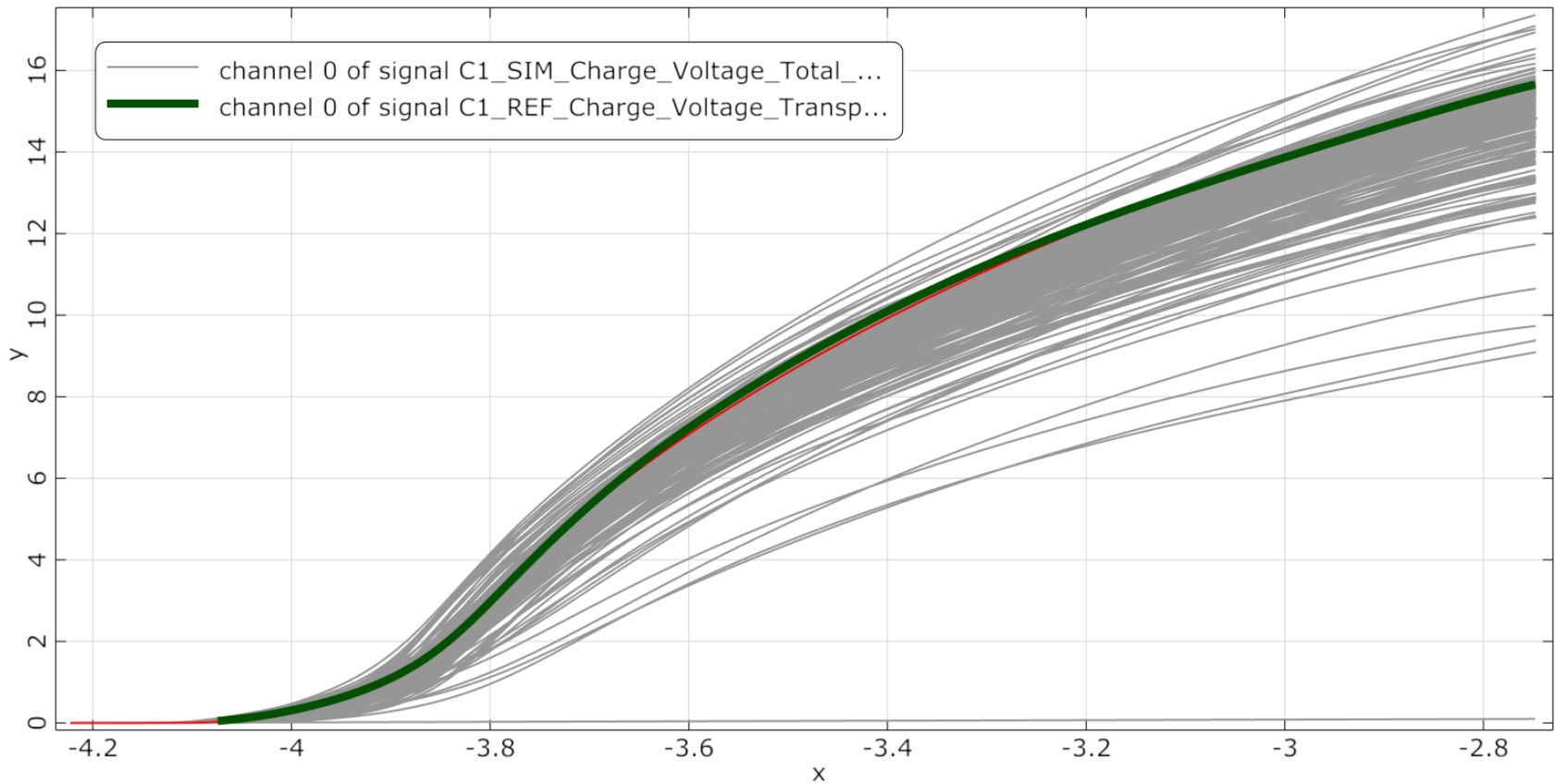




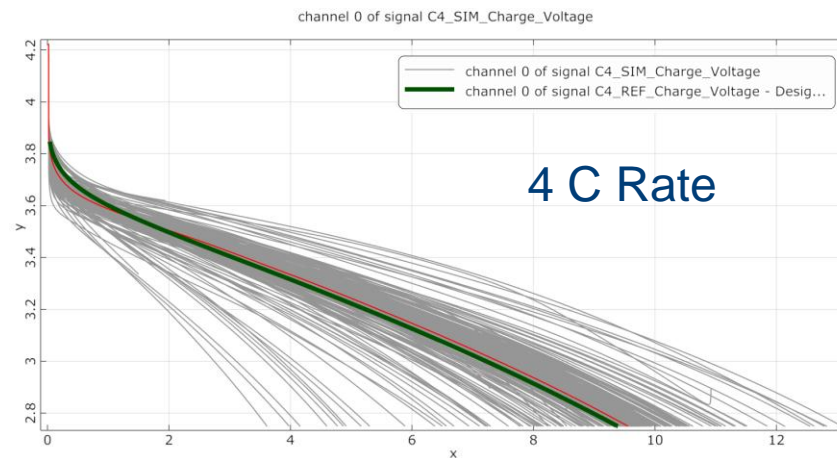
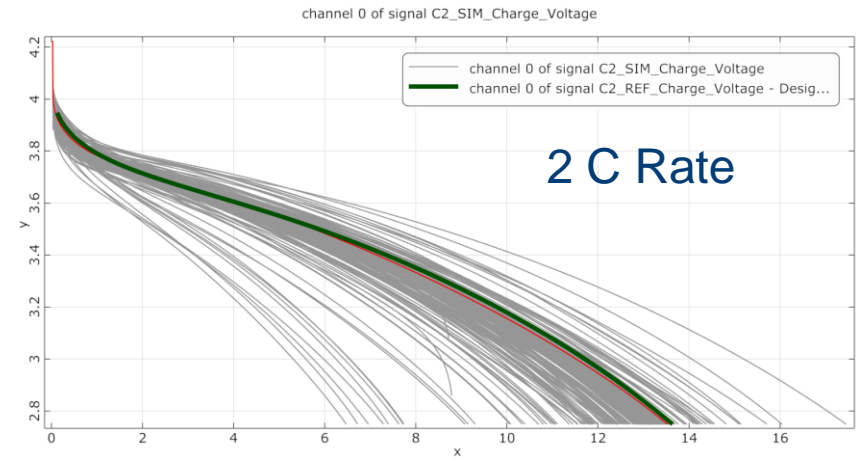
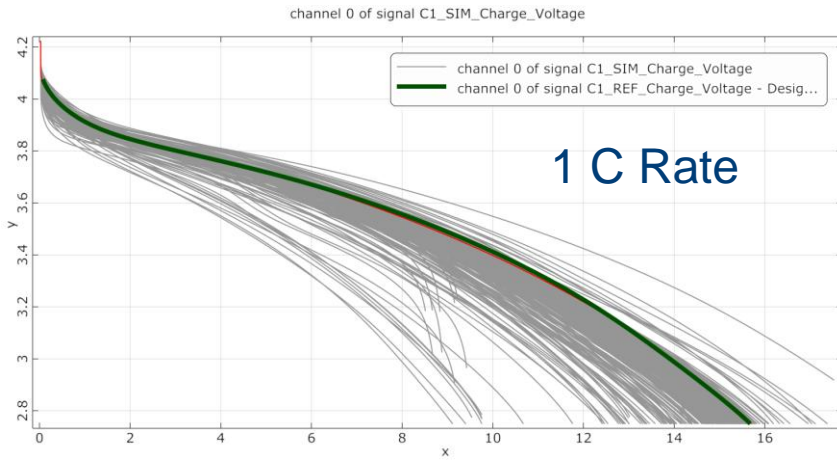
# Optimization Results

- Transposed 1 C Rate

channel 0 of signal C1\_SIM\_Charge\_Voltage\_Total\_Check\_Transposed



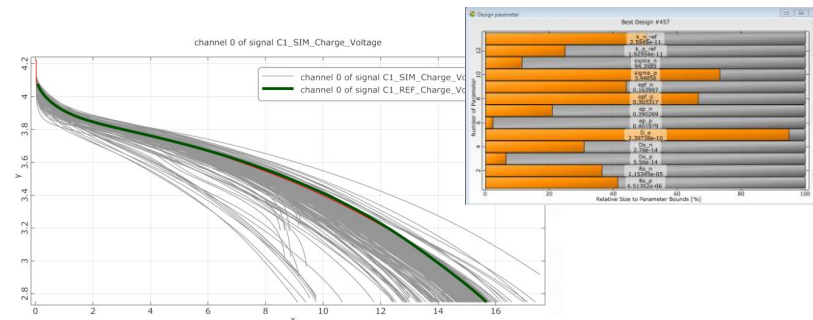
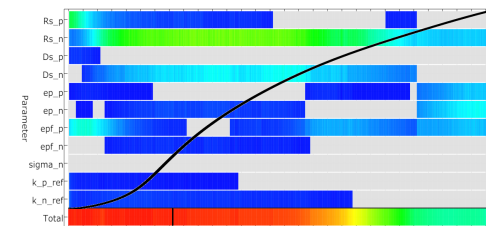
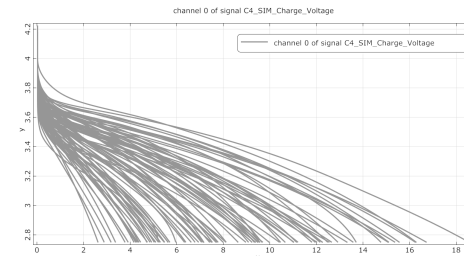
# Optimization Results





## 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



## Deutschland

**CADFEM GmbH**  
**Zentrale Grafing**  
Marktplatz 2  
85567 Grafing b. München  
T +49 (0) 8092 7005-0  
info@cadfem.de

**Geschäftsstelle Berlin**  
Breite Straße 2a  
13187 Berlin  
T +49 (0) 30 4759666-0

**Geschäftsstelle Dortmund**  
Hafenpromenade 1  
44263 Dortmund  
T +49 (0) 231 99325550

**Geschäftsstelle Hannover**  
Pelikanstraße 13  
30177 Hannover  
T +49 (0) 511 390603-0

**Geschäftsstelle Chemnitz**  
Schönherrstraße 8 / Eingang R  
09127 Chemnitz  
T +49 (0) 371 334262-0

**Geschäftsstelle Frankfurt**  
Im Kohlruß 5-7  
65835 Liederbach am Taunus  
T +49 (0) 6196 76708-0

**Geschäftsstelle Stuttgart**  
Leinfelder Straße 60  
70771 Leinfelden-Echterdingen  
T +49 (0) 711 990745-0

## Österreich

**CADFEM (Austria) GmbH**  
**Zentrale Wien**  
Wagenseilgasse 14  
1120 Wien  
T +43 (0) 1 5877073  
info@cadfem.at

**Geschäftsstelle Innsbruck**  
Grabenweg 3 (SOHO 2.0)  
6020 Innsbruck  
T +43 (0) 512 319056

## Schweiz

**CADFEM (Suisse) AG**  
**Zentrale Aadorf**  
Wittenwilerstrasse 25  
8355 Aadorf  
T +41 (0) 52 36801-01  
info@cadfem.ch

**Bureau Lausanne**  
Avenue de la Poste 3  
1020 Renens  
T +41 (0) 21 61480-40