LG Chem Meeting

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July 26, 2018

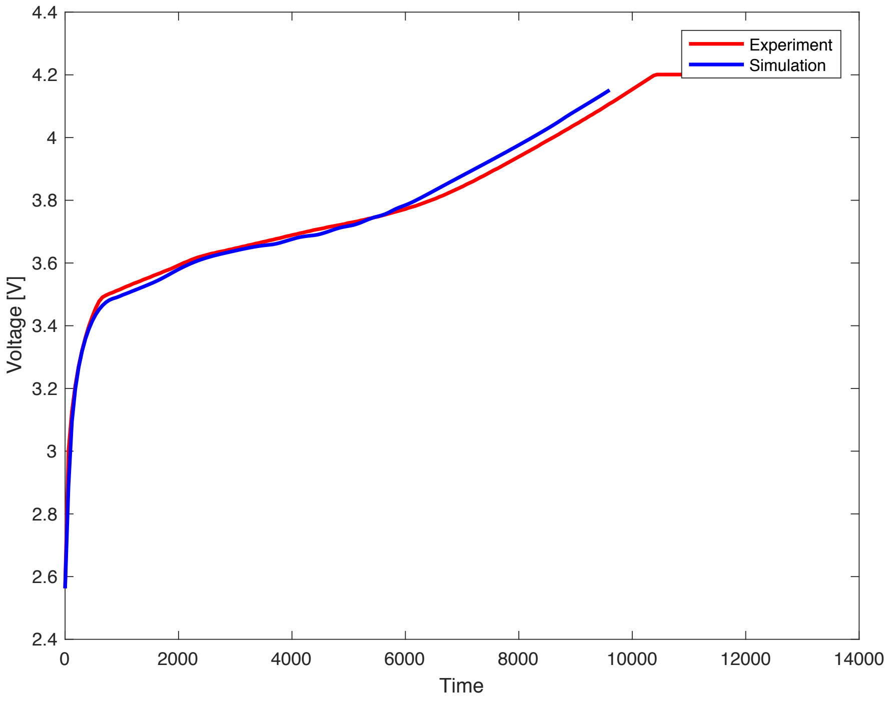
Agenda

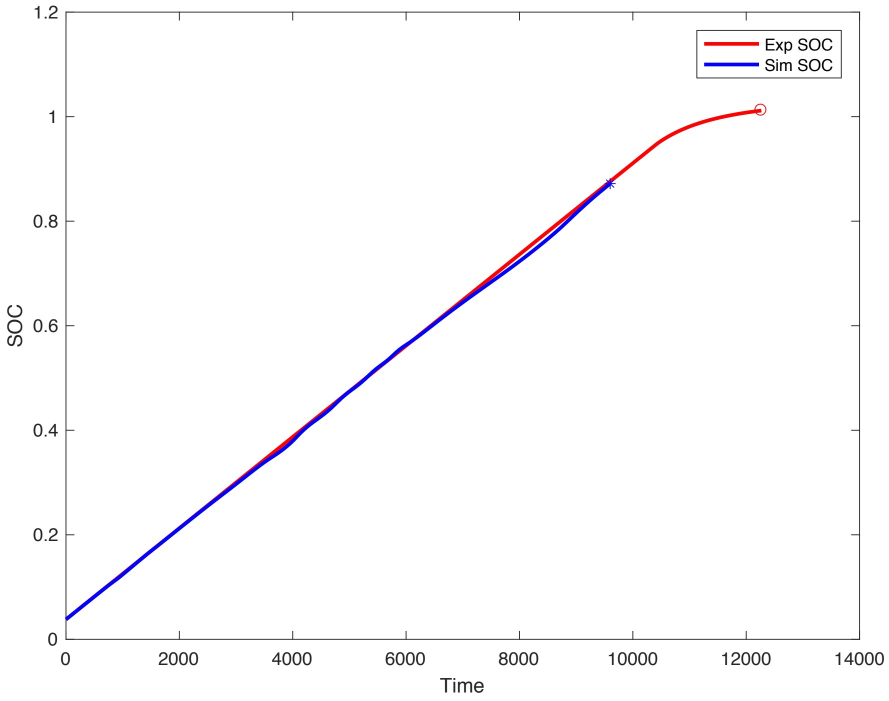
- **Full-order model validation**
  - Time-step effect
  - Exchange current density approximation

- **RL**
  - Understanding the best charge profile.
  - Reward function design

TimeStep Effect

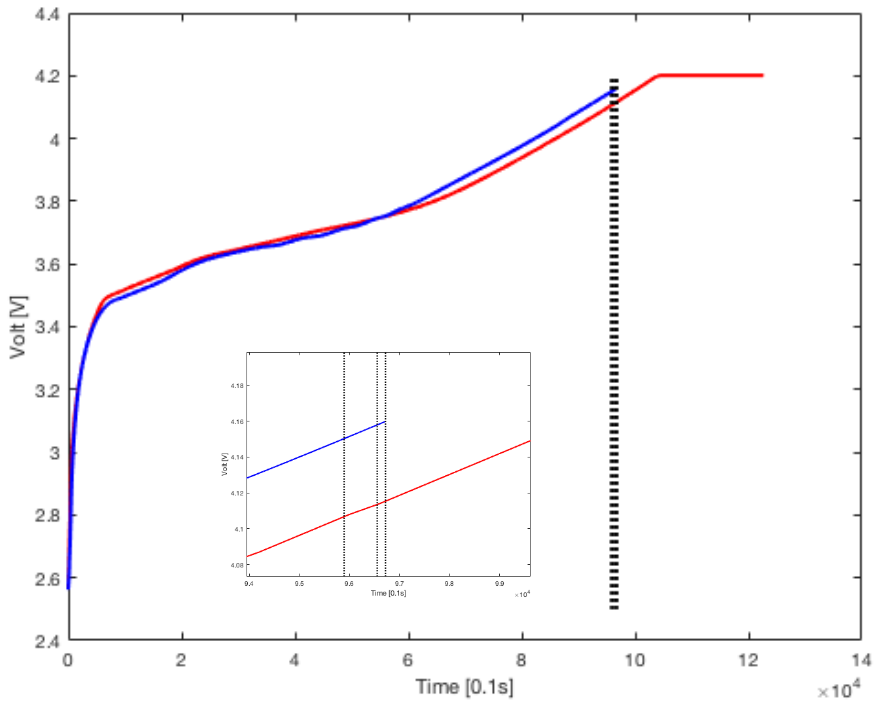
- **nodes (Anode/Sep/Cathode) along the x-axis**
  - 10/5/10
  - Ts=60s failed at 161 out of 206
- **Voltage / SOC**
  - Able to solve up to 85% SOC

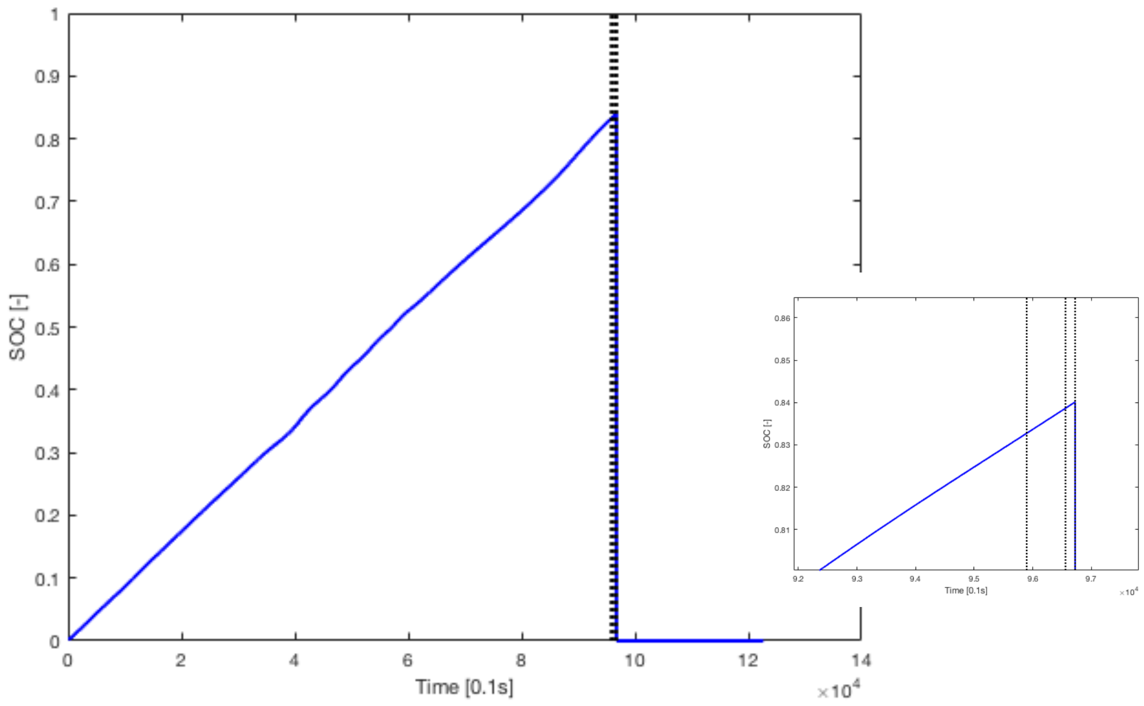




TimeStep Effect

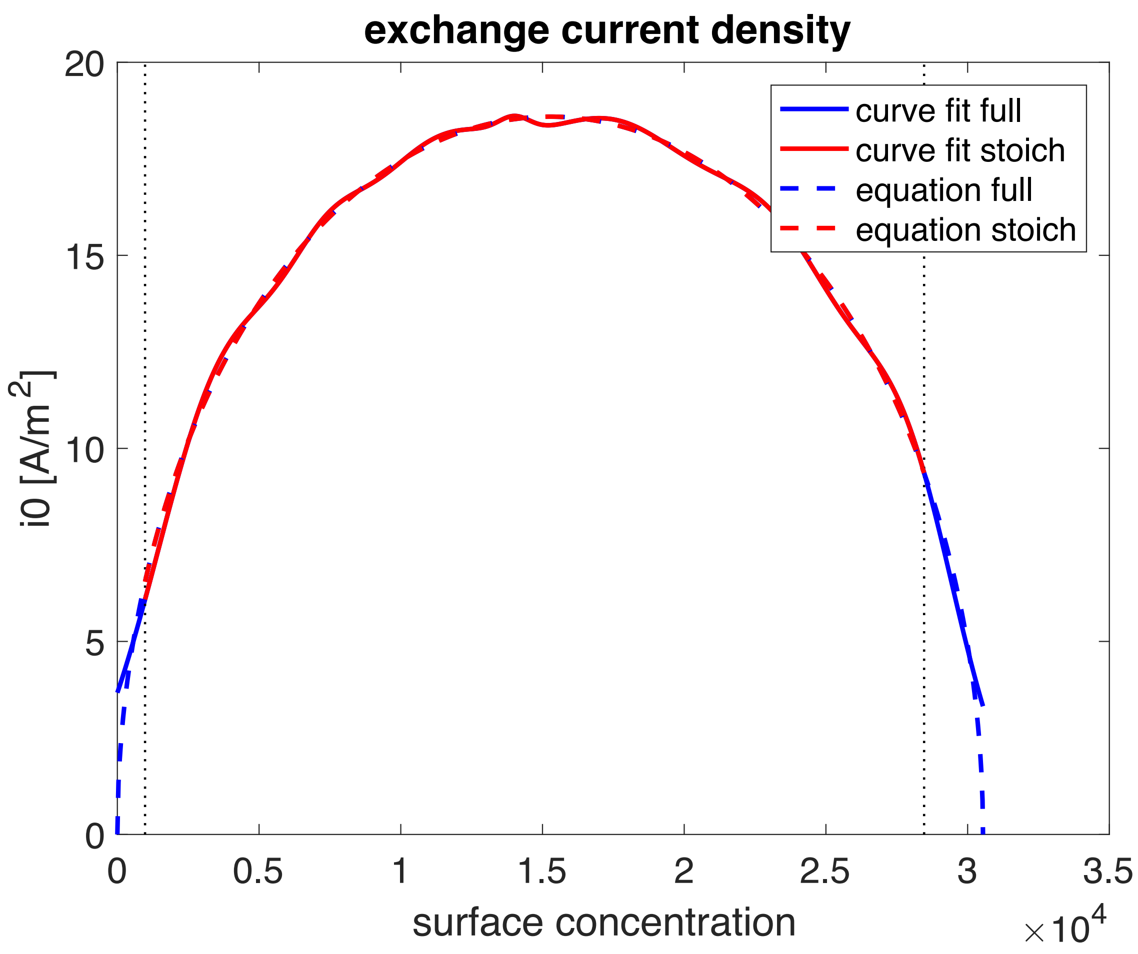
- **nodes (Anode/Sep/Cathode) along the x-axis**
  - 10/5/10
  - Ts=0.1s failed at 95896 out of 122668
  - Ts=0.01s failed at 96556 out of 122668
  - Ts=0.001s failed at 96722 out of 122668
- **Voltage / SOC**
  - With smaller time step we can compute 2% more SOC. (82->84% SoC)

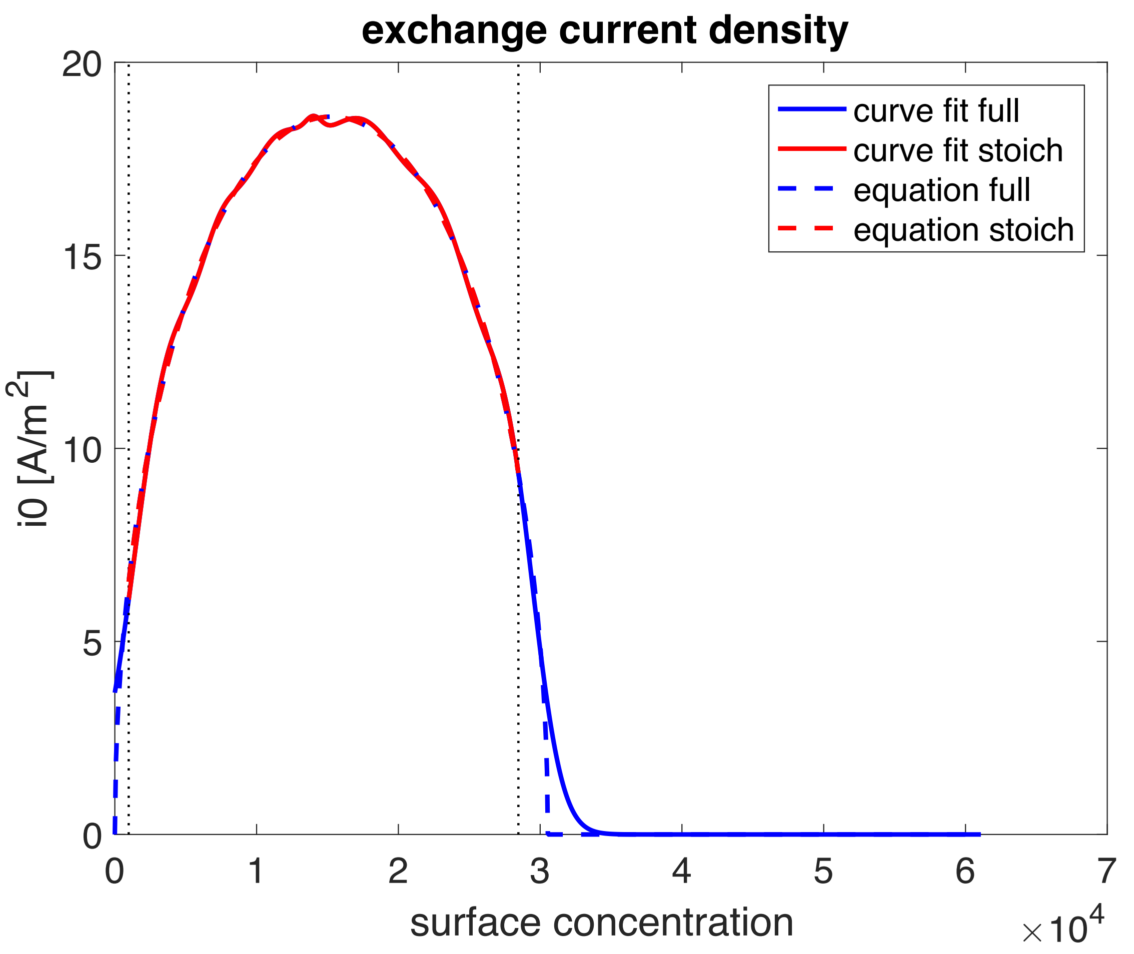




Function Fit

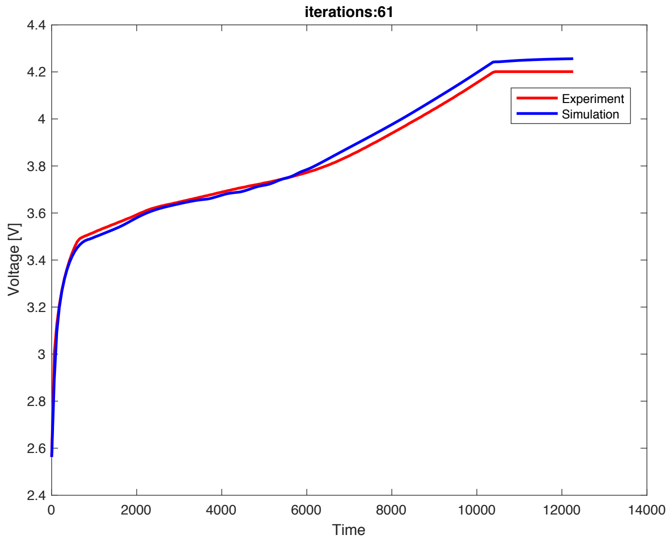
- **Function fit for c_ss_n term**
- **(left) within bound, (Right) without bound**

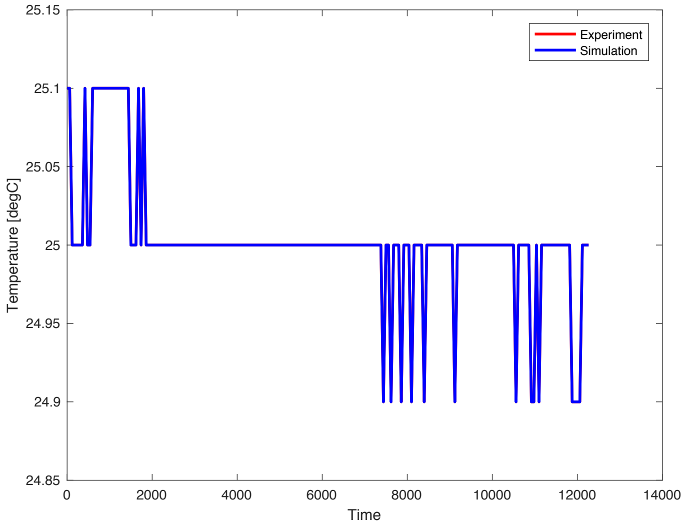


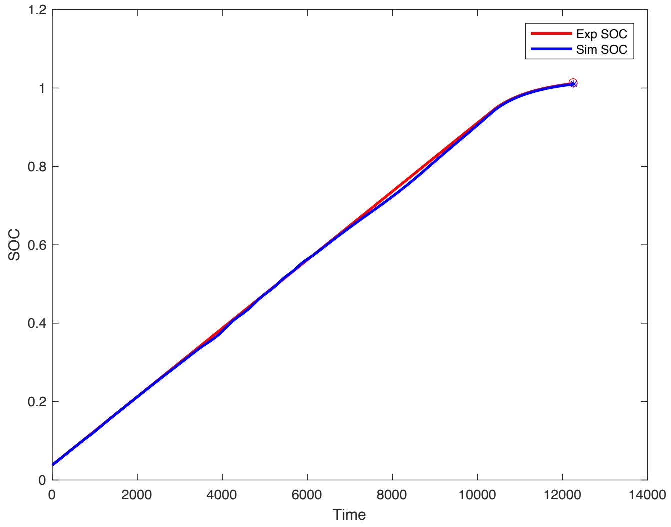


Validation

- **Input: current (0.3C CCCV), temperature**
  - Nodes for Anode/ Seperator / Cathode = 10/5/10
  - 32.2mV RMSE
  - 0 degC RMSE
  - 57.1E-05 SoC RMSE.

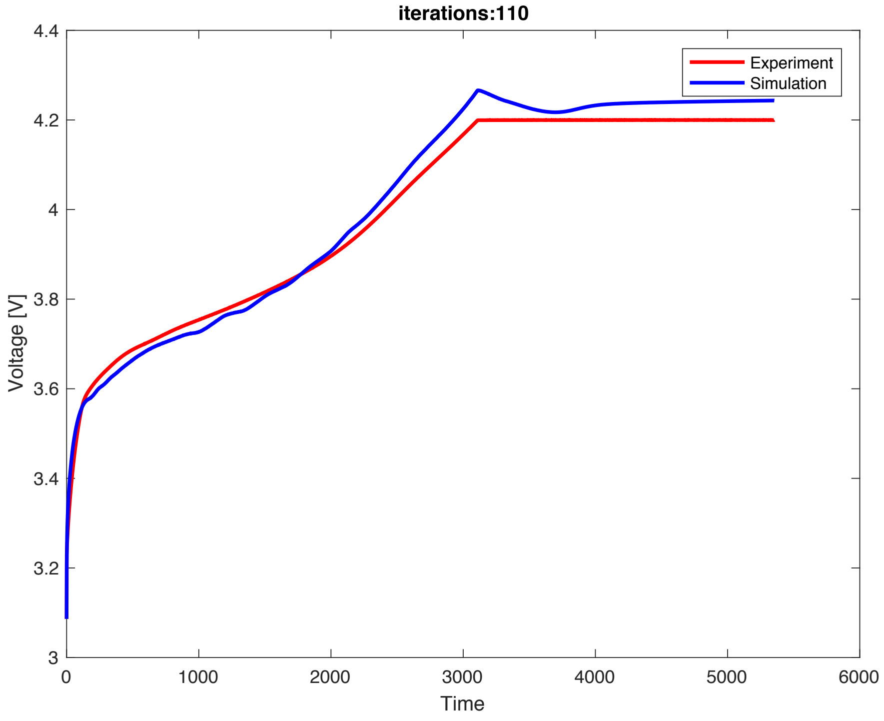


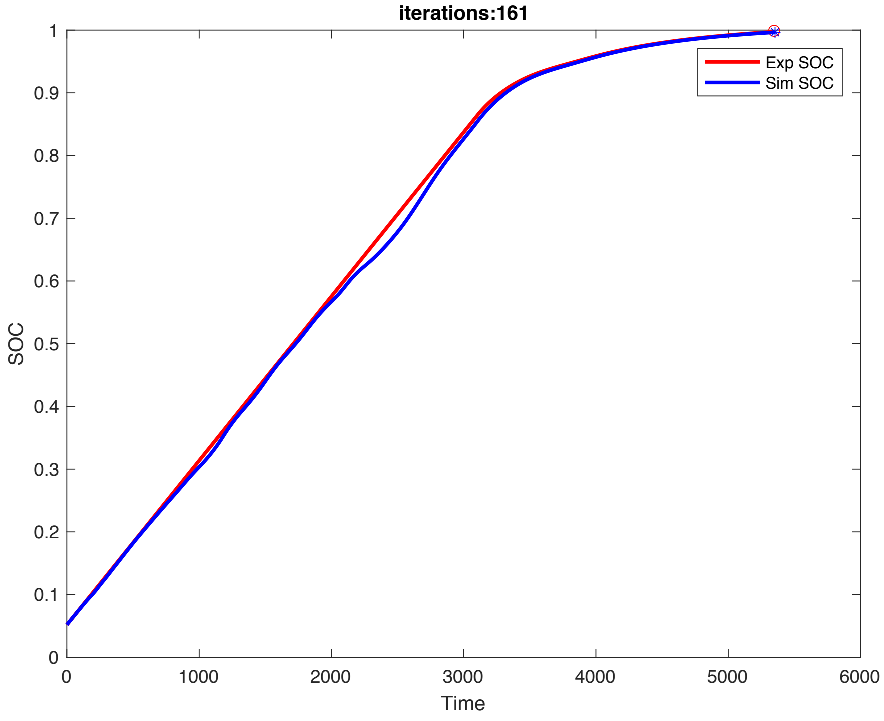




Validation

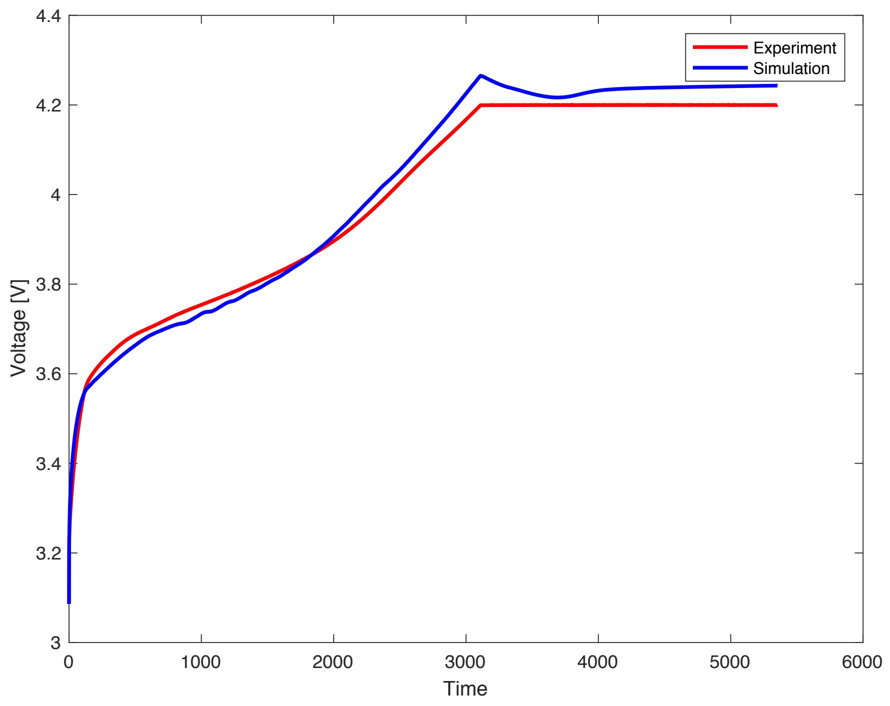
- **Input: current (1C CCCV), temperature**
  - Nodes for Anode/ Seperator / Cathode = 10/5/10
  - 33.4mV RMSE
  - 92.9E-04 SoC RMSE.

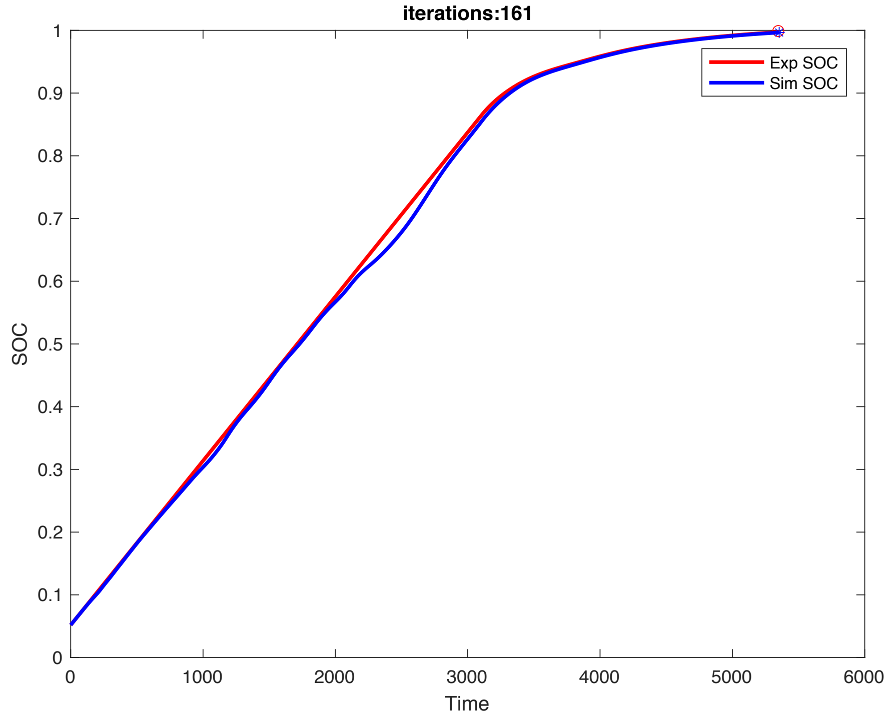




Validation

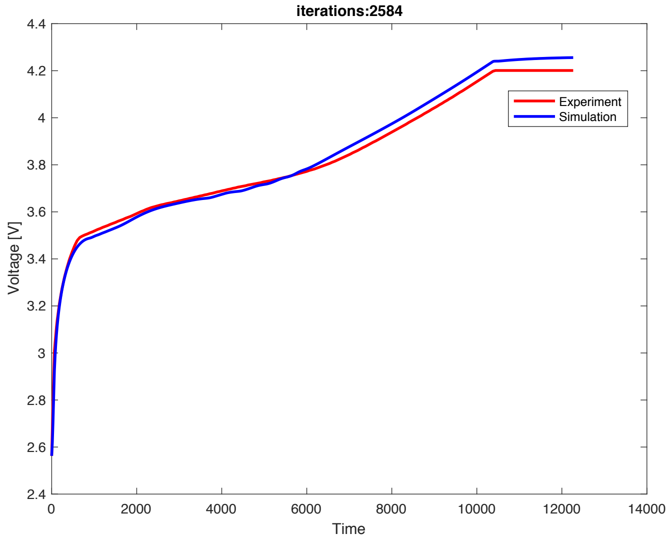
- **Input: current (1C CCCV), temperature**
  - Nodes for Anode/ Seperator / Cathode = 20/10/20
  - 33.4mV RMSE
  - 96.9E-04 SoC RMSE.

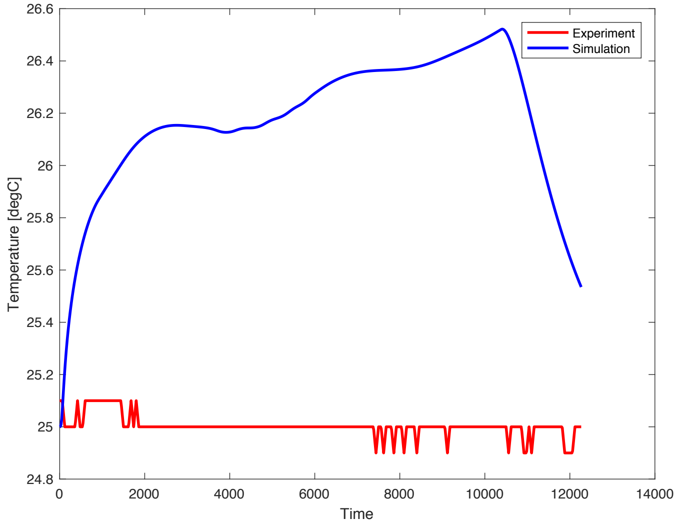


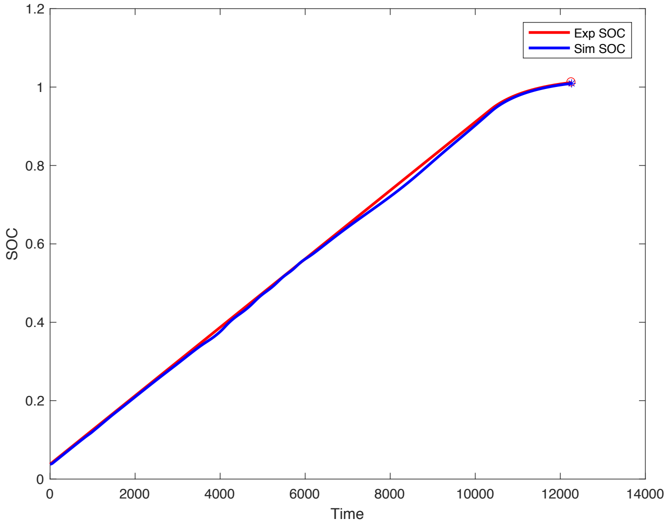


Validation

- **Input: current (0.3C CCCV)**
  - Nodes for Anode/ Separator / Cathode = 10/5/10
  - TimeStep = 0.1sec
  - 31.1mV RMSE
  - 1.19degC RMSE
  - 76.6E-04 SoC RMSE.

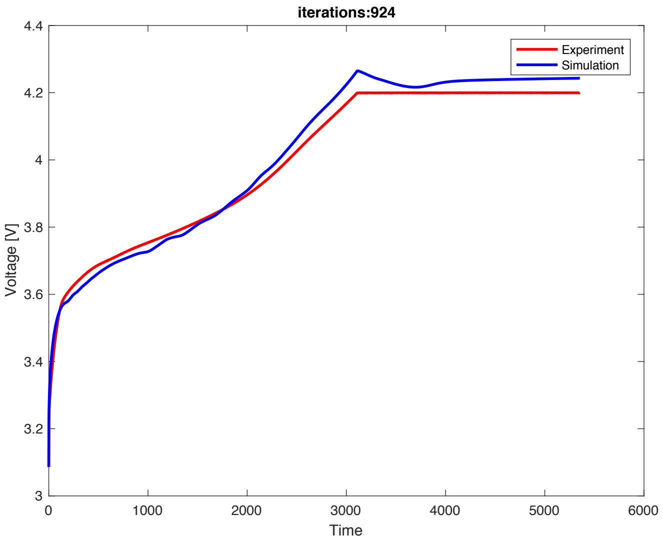


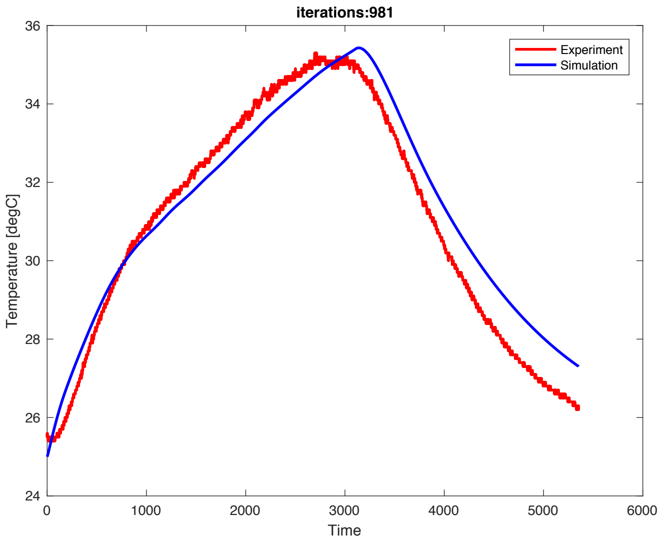


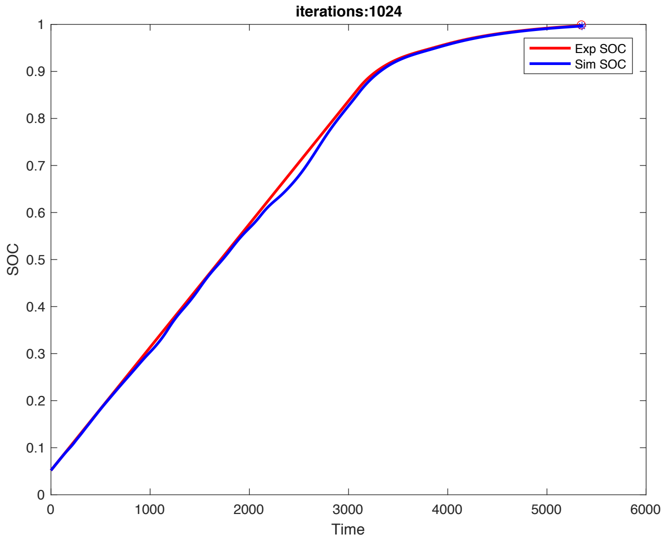


Validation

- **Input: current (1C CCCV)**
  - Nodes for Anode/ Separator / Cathode = 10/5/10
  - 33.3mV RMSE
  - 0.734degC RMSE
  - 92.6E-04 SoC RMSE.

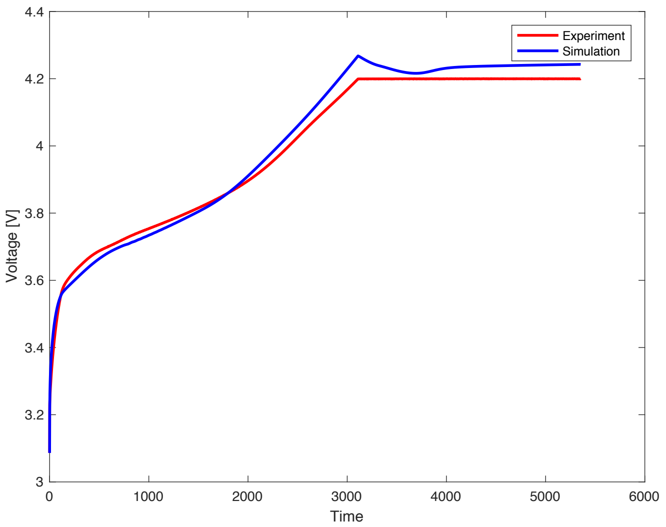


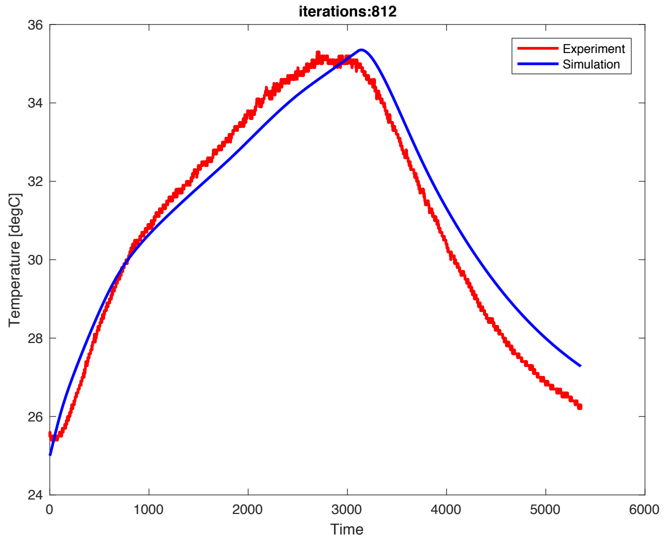


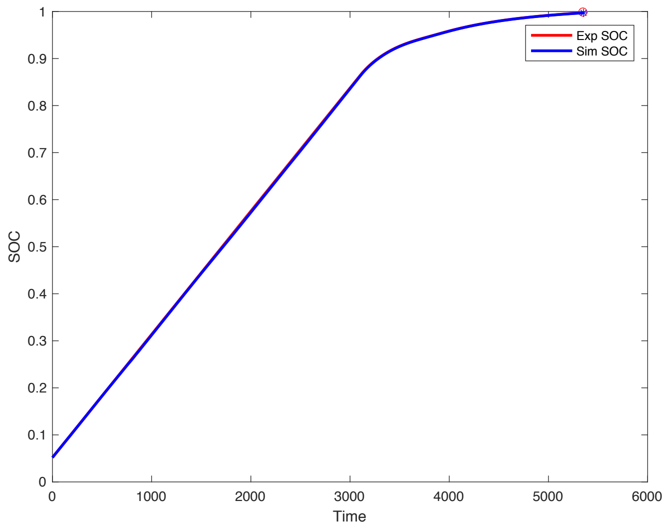


Validation

- **Input: current (1C CCCV)**
  - Nodes for Anode/ Separator / Cathode = 70/35/70
  - 32.6mV RMSE
  - 0.717degC RMSE
  - 13.6E-04 SoC RMSE.







Summary

- **RMSE $\leq$ 40mV | RMSE $\leq$ 0.1% SoC | RMSE $\leq$ 1.5degC**

- **TimeStep effect**
  - Small-time step helps to solve numerical problems, but still issues remain.
  - Approximating current density function is recommended.

- **Discretization effect**
  - Small number of discretization helps fast simulation.
  - Notably, RMSE of SOC increases as number of discretization reduces.

- **RL framework**
  - Reinforcement learning requires a very **high volume** of "trial and error" episodes - or interactions with an environment.
  - In order to learn a good policy, simulators are required to achieve results in a cost-effective and timely way.

- **Suggestions for environment design**
  - Use approximated current density function
  - Sample time = 1sec
  - Use 10/5/10 nodes for simulation environment

Need to validate higher C-rates with 1sec timestep

Optimal Charging problem

- **Minimum charging**
  - Fast charge
  - Suppress aging

$$\underset{\boldsymbol{I(t)}}{\mathbf{arg}\min} \int_{\mathbf{0}}^{\boldsymbol{t_f}} \mathbf{1}\boldsymbol{dt}$$

subject to:

Battery eqns

input constraints (magnitude, capacity)

state constraints (Temperature, Overpotential)

- **Max charge throughput**
  - Finite amount of time, charge battery up to certain point

- **Least square of target SoC and current SoC.**
  - Charge battery up to target SoC

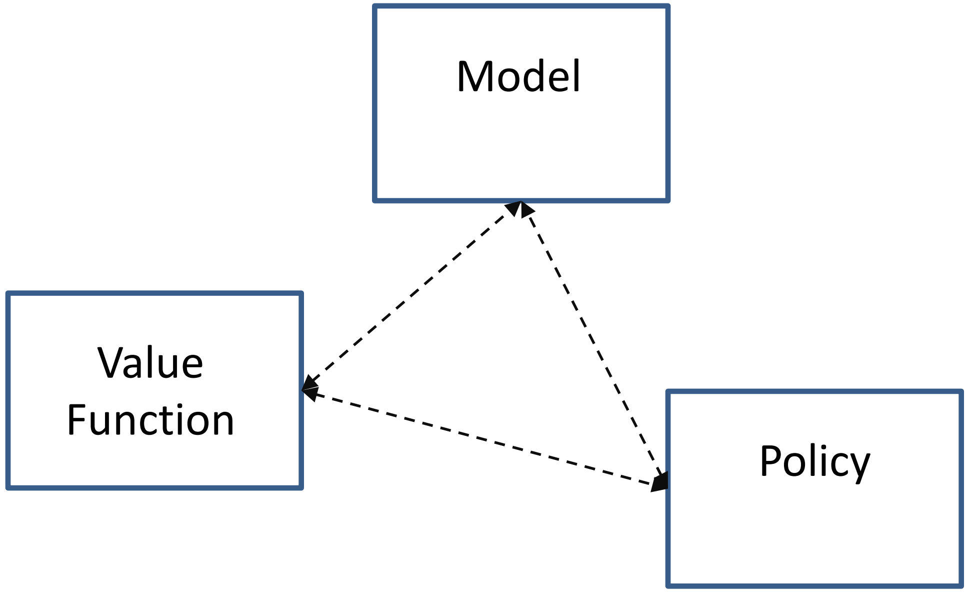
There are many optimal charging problems!

Reinforcement learning framework

- **RL Background**
  - Markov Decision Process (MDP)
  - Dynamic Programming
    - Value Iteration
    - Policy Iteration
  - Policy Optimization
    - Policy gradients

- **RL algorithms**
  - DQN (Deep Q Network)
  - DPG (Deterministic Policy gradient)
  - A3C (Asynchronous Advantage Actor-Critic)

- **Model**
  - Control Sys | Machine Learning
    - Model-based RL : Train network to predict ‘state transition’ and reward models
    - Model-free RL : Not try to learn explicit models of the env.
    - We focus on ‘Model-free RL’ for ‘model-based’ control



- Value function
  - State-value function
  - State-action function
- Policy

RL problem formulation

- **Minimum time charging.**
  - Maximize negative rewards

  - Violate constraints -> episode is over
    - Surface concentrations
    - Electrolyte concentrations
    - Temperature

- **Basic sketch**
  - From fixed initial point, we reach certain stage of charging without violating constraints